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NEWS	1		Web Page for STN Seminar Schedule - N. America
NEWS	2	JUL 28	CA/CAPplus patent coverage enhanced
NEWS	3	JUL 28	EPFULL enhanced with additional legal status information from the epline Register
NEWS	4	JUL 28	IFICDB, IFIPAT, and IFIUDB reloaded with enhancements
NEWS	5	JUL 28	STN Viewer performance improved
NEWS	6	AUG 01	INPADOCDB and INPAFAMDB coverage enhanced
NEWS	7	AUG 13	CA/CAPplus enhanced with printed Chemical Abstracts page images from 1967-1998
NEWS	8	AUG 15	CAOLD to be discontinued on December 31, 2008
NEWS	9	AUG 15	CAPplus currency for Korean patents enhanced
NEWS	10	AUG 27	CAS definition of basic patents expanded to ensure comprehensive access to substance and sequence information
NEWS	11	SEP 18	Support for STN Express, Versions 6.01 and earlier, to be discontinued
NEWS	12	SEP 25	CA/CAPplus current-awareness alert options enhanced to accommodate supplemental CAS indexing of exemplified prophetic substances
NEWS	13	SEP 26	WPIDS, WPINDEX, and WPIX coverage of Chinese and Korean patents enhanced
NEWS	14	SEP 29	IFICLS enhanced with new super search field
NEWS	15	SEP 29	EMBASE and EMBAL enhanced with new search and display fields
NEWS	16	SEP 30	CAS patent coverage enhanced to include exemplified prophetic substances identified in new Japanese-language patents
NEWS	17	OCT 07	EPFULL enhanced with full implementation of EPC2000
NEWS	18	OCT 07	Multiple databases enhanced for more flexible patent number searching
NEWS	19	OCT 22	Current-awareness alert (SDI) setup and editing enhanced
NEWS	20	OCT 22	WPIDS, WPINDEX, and WPIX enhanced with Canadian PCT Applications
NEWS	21	OCT 24	CHEMLIST enhanced with intermediate list of pre-registered REACH substances
NEWS EXPRESS	JUNE 27 08		CURRENT WINDOWS VERSION IS V8.3, AND CURRENT DISCOVER FILE IS DATED 23 JUNE 2008.
NEWS HOURS			STN Operating Hours Plus Help Desk Availability
NEWS LOGIN			Welcome Banner and News Items
NEWS IPC8			For general information regarding STN implementation of IPC 8

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                              ENTRY      SESSION
FULL ESTIMATED COST          0.21      0.21
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STRUCTURE FILE UPDATES: 24 OCT 2008 HIGHEST RN 1065816-63-8  
DICTIONARY FILE UPDATES: 24 OCT 2008 HIGHEST RN 1065816-63-8

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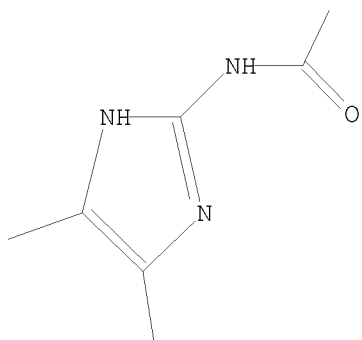
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Uploading C:\Program Files\STNEXP\Queries\10564010 str 2.str

L1 STRUCTURE UPLOADED

=> que L1

L2 QUE L1

=> d l2  
L2 HAS NO ANSWERS  
L1 STR



Structure attributes must be viewed using STN Express query preparation.  
 L2 QUE ABB=ON PLU=ON L1

=> s l2 sss full  
 FULL SEARCH INITIATED 11:30:59 FILE 'REGISTRY'  
 FULL SCREEN SEARCH COMPLETED - 1577 TO ITERATE

100.0% PROCESSED 1577 ITERATIONS 22 ANSWERS  
 SEARCH TIME: 00.00.01

L3 22 SEA SSS FUL L1

=> file caplus		
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	ENTRY	SESSION
FULL ESTIMATED COST	178.36	178.57

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FILE COVERS 1907 - 27 Oct 2008 VOL 149 ISS 18  
 FILE LAST UPDATED: 26 Oct 2008 (20081026/ED)

Caplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2008.

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

<http://www.cas.org/legal/infopolicy.html>

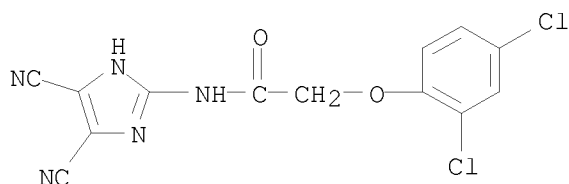
=> s l3

L4 22 L3  
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25113423 PY<=2004  
L5 16 L4 AND PY<=2004  
=> d 15 1-16 ibib ab hitstr

L5 ANSWER 1 OF 16 CAPLUS COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 2003:836594 CAPLUS  
DOCUMENT NUMBER: 139:323523  
TITLE: Preparation of aryloxycarbamoylazoles as calcium  
channel blockers  
INVENTOR(S): Snutch, Terrance P.  
PATENT ASSIGNEE(S): Can.  
SOURCE: U.S. Pat. Appl. Publ., 22 pp.  
CODEN: USXXCO  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20030199523	A1	20031023	US 2003-377090	20030228 <--
PRIORITY APPLN. INFO.:			US 2002-360917P	P 20020228

OTHER SOURCE(S): MARPAT 139:323523  
AB ArXQ, Ar2CHXQ [Ar = 6-membered (substituted) aryl containing  $\geq 1$  S, O and N, optionally coupled through O to the linker X; X = (substituted) alkylene of 2-10 sequentially connected atoms selected from C, N, O, and S; Q = 5-membered (substituted) heterocyclyl containing  $\geq 1$  N or S atom], were prepared Thus, O-benzotriazolyl-N,N,N',N'-tetramethyluronium tetrafluoroborate was added to a solution of 2-(4,4'-dichlorobenzhydryl)acetic acid, 2-amino-5-nitrothiazole, and Et3N in CH2Cl2/MeCN and the reaction mixture was stirred at room temperature overnight to give N-2-(5-nitrothiazolyl)-2-(4,4'-dichlorobenzhydryl)acetic amide (NT 051). NT 051 blocked  $\alpha 1B$ ,  $\alpha 1A$ , and  $\alpha 1C$  channels with IC50 = 0.13  $\mu M$ , 6.8  $\mu M$ , and 1.91  $\mu M$ , resp.  
IT 615283-83-5  
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
(preparation of aryloxycarbamoylazoles as calcium channel blockers)  
RN 615283-83-5 CAPLUS  
CN Acetamide, 2-(2,4-dichlorophenoxy)-N-(4,5-dicyano-1H-imidazol-2-yl)- (CA INDEX NAME)



L5 ANSWER 2 OF 16 CAPLUS COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 2003:532641 CAPLUS  
DOCUMENT NUMBER: 139:101147

TITLE: Preparation of aromatic hydrocarbon-fused heterocyclic dithiols and disulfides as electron-accepting compounds capable of forming self-assembled monolayers

INVENTOR(S): Saso, Haruo; Satoh, Toshiaki; Takahashi, Toshiaki; Ogawa, Satoshi; Yoshimoto, Noriyuki

PATENT ASSIGNEE(S): Nippon Soda Co., Ltd., Japan

SOURCE: PCT Int. Appl., 54 pp.  
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003055853	A1	20030710	WO 2002-JP13590	20021226 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2002357515	A1	20030715	AU 2002-357515	20021226 <--
PRIORITY APPLN. INFO.:				
			JP 2001-394984	A 20011226
			JP 2002-40385	A 20020218
			WO 2002-JP13590	W 20021226

OTHER SOURCE(S): MARPAT 139:101147

AB The compds. represented by the general formula A-Sp-X [wherein A is (i) an aromatic heterocyclic group bearing at least one member selected from the group consisting of cyano, C1-6 alkoxy carbonyl, and C1-11 acyl either on the ring or in a state attached to the ring through a conjugated system or (ii) an electron-accepting functional group to which at least one aromatic hydrocarbon ring is fused; Sp is a divalent connecting group containing an arylene group and/or an alkylene group; and X is a binding group capable of making a connection to a metal surface, a metal oxide surface, or a semiconductor surface by a covalent or coordinate bond] are prepared. These Compds. have simple structures and are easy of preparation and have the ability to accept an electron and can be self-assembled to form monolayers easily. They are useful as raw materials for mol. devices. Thus, a mixture of naphthalene-1,4,5,8-tetracarboxylic acid dianhydride 5.36, 5-hydroxy-1-pentylamine 4.54, p-toluenesulfonic acid 0.19 g, and 100 mL toluene was refluxed for 8 h with removing H<sub>2</sub>O though a Dean Stark trap to give 87% N,N'-bis(5-hydroxypentyl)-1,4,5,8-naphthalenetetracarboxylic diimide (I). I (2.02 g) and 3.26 g PBr<sub>3</sub> were refluxed in the presence of a catalytic amount of pyridine in 100 mL toluene for 7 h to give 2.65 g crude N,N'-bis(5-bromopentyl)-1,4,5,8-naphthalenetetracarboxylic diimide which was dissolved in 50 mL CHCl<sub>3</sub>, successively treated with 1.66 g Bu<sub>4</sub>NBr and aqueous solution of 1.30 g potassium thiosulfate in 20 mL H<sub>2</sub>O and stirred at room temperature for 25 h to give 81% N,N'-bis(5-acetylthiopentyl)-1,4,5,8-naphthalenetetracarboxylic diimide (II). II (3.21 g) was suspended in 100 MeOH, treated with 10 mL concentrated HCl, and heated under refluxed for 7 days to give 29% N,N'-bis(5-mercaptopentyl)-1,4,5,8-naphthalenetetracarboxylic diimide (III). A gold electrode (1.6 mm diameter) for cyclic voltammetry was immersed in 0.1 mM III/EtOH for 24 h, and successively washed with ethanol and MeCN. A reduction potential of -1.33 V was observed using a Ag/AgNO<sub>3</sub> reference

electrode and a Pt electrode against the gold electrode prepared above, which confirmed the formation of a thin film on the gold surface.

IT 556815-13-5P

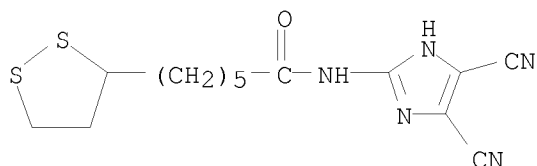
RL: DEV (Device component use); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)

(preparation of aromatic hydrocarbon-fused heterocyclic dithiols and disulfides

as electron-accepting compds. capable of forming self-assembled monolayers)

RN 556815-13-5 CAPLUS

CN 1,2-Dithiolane-3-hexanamide, N-(4,5-dicyano-1H-imidazol-2-yl)- (CA INDEX NAME)



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 3 OF 16 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2002:888725 CAPLUS

DOCUMENT NUMBER: 137:384838

TITLE: Heterocycle-substituted amides as protease inhibitors

INVENTOR(S): Cardel, Bettina; Metz, Guenther; Ottleben, Holger; Rau, Harald; Schellhaas, Nathalie; Sekul, Renate; Vetter, Dirk; Bode, Wolfram; Friedrich, Rainer

PATENT ASSIGNEE(S): Graffinity Pharmaceuticals A.-G., Germany

SOURCE: PCT Int. Appl., 180 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002092582	A1	20021121	WO 2002-EP5369	20020515 <--
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
DE 10124041	A1	20021121	DE 2001-10124041	20010516 <--
AU 2002304630	A1	20021125	AU 2002-304630	20020515 <--
EP 1387833	A1	20040211	EP 2002-732716	20020515 <--
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR			
PRIORITY APPLN. INFO.:			DE 2001-10124041	A 20010516
			WO 2002-EP5369	W 20020515

OTHER SOURCE(S): MARPAT 137:384838

AB ADCR1R2COXCHYEZ [A = (un)substituted aryl, cycloalkyl, cycloalkenyl; D =

O, S, S(O), SO<sub>2</sub>; R<sub>1</sub>, R<sub>2</sub> = NO<sub>2</sub>, (un)substituted alkyl, alkoxy, acyl, alkoxy carbonyl, acyloxy, NH<sub>2</sub>, CONH<sub>2</sub>, cycloalkyl, aryl, benzyl; X = O, S, (un)substituted NH; Y = (un)substituted aryl, cycloalkyl, cycloalkenyl, alkyl, alkoxy, acyl; E, Z = H, F, Cl, Br, I, OH, SH, CF<sub>3</sub>, NO<sub>2</sub>, acyl, (un)substituted CO<sub>2</sub>H, acyloxy, alkyl, alkoxy, NH<sub>2</sub>, CONH<sub>2</sub>, aryl, cycloalkyl, cycloalkenyl, bicycloalkenyl; EZ = (un)substituted CONH<sub>2</sub>] were prepared for use as inhibitors of proteases, especially serine proteases such

as

thrombin. Thus, the diamide I was prepared from polymer-supported 4-H<sub>2</sub>NSO<sub>2</sub>C<sub>6</sub>H<sub>4</sub>CO<sub>2</sub>H, N-9-fluorenylmethoxycarbonyl-L-4-thiazolylalanine, 4-ClC<sub>6</sub>H<sub>4</sub>SCH<sub>2</sub>CO<sub>2</sub>H, and histamine by solid-phase synthesis. I had K<sub>i</sub> for inhibition of thrombin activity of 6X10<sup>-6</sup> M.

IT 475680-12-7P

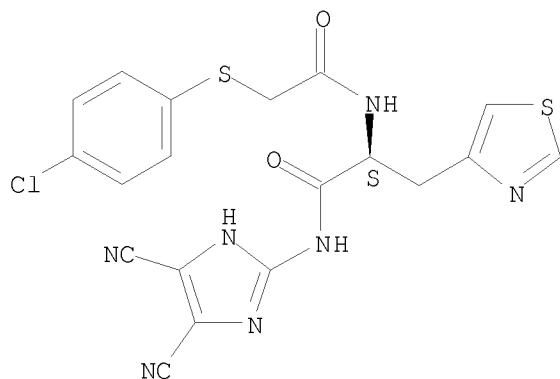
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of heterocycle-substituted amides as inhibitors of thrombin and factor X)

RN 475680-12-7 CAPLUS

CN 4-Thiazolepropanamide, α-[[2-[(4-chlorophenyl)thio]acetyl]amino]-N-(4,5-dicyano-1H-imidazol-2-yl)-, (αS)- (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 4 OF 16 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2002:855867 CAPLUS

DOCUMENT NUMBER: 139:214346

TITLE: Product class 3: imidazoles

AUTHOR(S): Grimmett, M. R.

CORPORATE SOURCE: Organic Chemistry, Dept. of Chemistry, University of Otago, Dunedin, N. Z.

SOURCE: Science of Synthesis (2002), 12, 325-528  
CODEN: SSCYJ9

PUBLISHER: Georg Thieme Verlag

DOCUMENT TYPE: Journal; General Review

LANGUAGE: English

AB A review. Methods for preparing imidazoles are reviewed including cyclization, ring transformations, aromatization and modification of substituents on existing imidazoles.

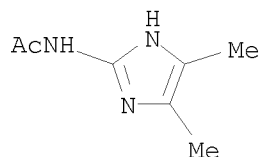
IT 40639-97-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of imidazoles via cyclization, ring transformation, aromatization and substituent modifications)

RN 40639-97-2 CAPLUS

CN Acetamide, N-(4,5-dimethyl-1H-imidazol-2-yl)- (CA INDEX NAME)



REFERENCE COUNT: 823 THERE ARE 823 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 5 OF 16 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2002:827797 CAPLUS

DOCUMENT NUMBER: 137:331022

TITLE: Coupler for azomethine dye formation and silver halide photographic material using it

INVENTOR(S): Ogasawara, Atsushi; Kamihira, Shigeo; Shimada, Yasuhiro

PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 28 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2002318441	A	20021031	JP 2001-123651	20010420 <--
PRIORITY APPLN. INFO.:			JP 2001-123651	20010420

OTHER SOURCE(S): MARPAT 137:331022

AB Dye forming coupler I and azomethine dye II (Q = nonmetal atoms to form N-containing heterocycle; R = substituent; Het = heterocycle; X = H, releasing group by coupling reaction with developer oxide; Ar = aryl) are claimed. The azomethine dye shows high mol. extinction coeff, clear hue, and the photog. material gives clear images with good fastness.

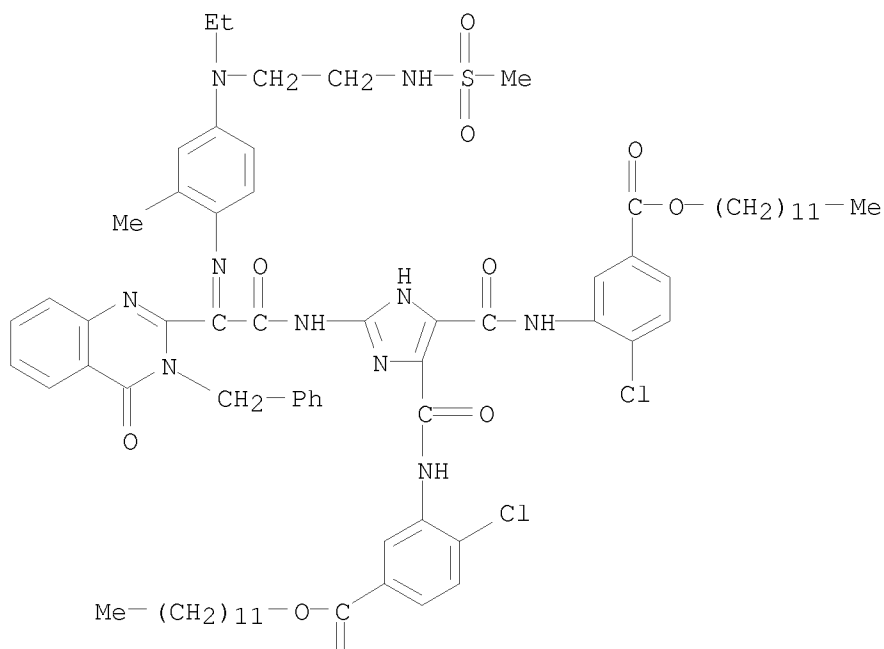
IT 473738-67-9P

RL: PNU (Preparation, unclassified); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

(azomethine dye; photog. coupler for azomethine dye formation)

RN 473738-67-9 CAPLUS

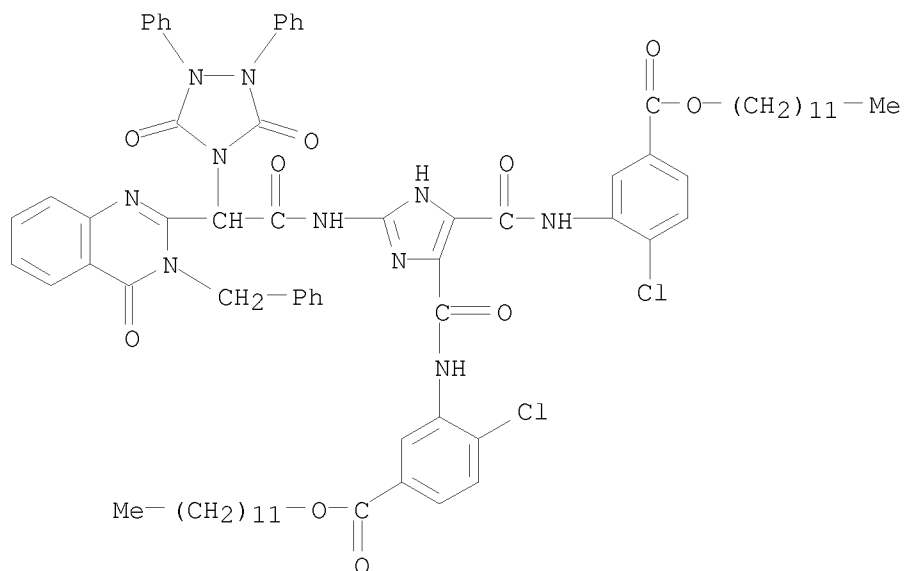
CN Benzoic acid, 3,3'-[[2-[[[3,4-dihydro-4-oxo-3-(phenylmethyl)-2-quinazolinyl][4-[ethyl[2-[(methylsulfonyl)amino]ethyl]amino]-2-methylphenyl]imino]acetyl]amino]-1H-imidazole-4,5-diyl]bis(carbonylimino)]bis[4-chloro-, didodecyl ester (9CI) (CA INDEX NAME)



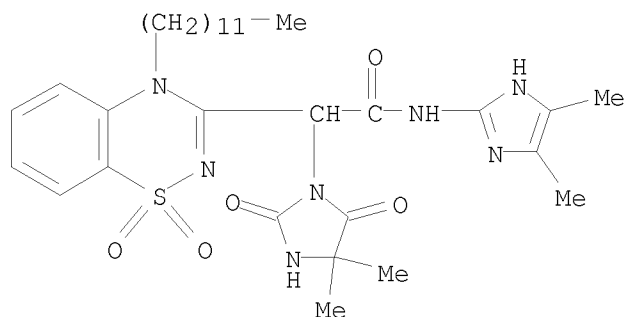
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IT      473738-53-3P
      RL: PNU (Preparation, unclassified); RCT (Reactant); TEM (Technical or
      engineered material use); PREP (Preparation); RACT (Reactant or reagent);
      USES (Uses)
          (photog. coupler for azomethine dye formation)
RN      473738-53-3  CAPLUS
CN      Benzoic acid, 3,3'-[[2-[[[3,4-dihydro-4-oxo-3-(phenylmethyl)-2-
      quinazolinyl](3,5-dioxo-1,2-diphenyl-1,2,4-triazolidin-4-yl)acetyl]amino]-
      1H-imidazole-4,5-diyl]bis(carbonylimino)]bis[4-chloro-, didodecyl ester
      (9CI) (CA INDEX NAME)

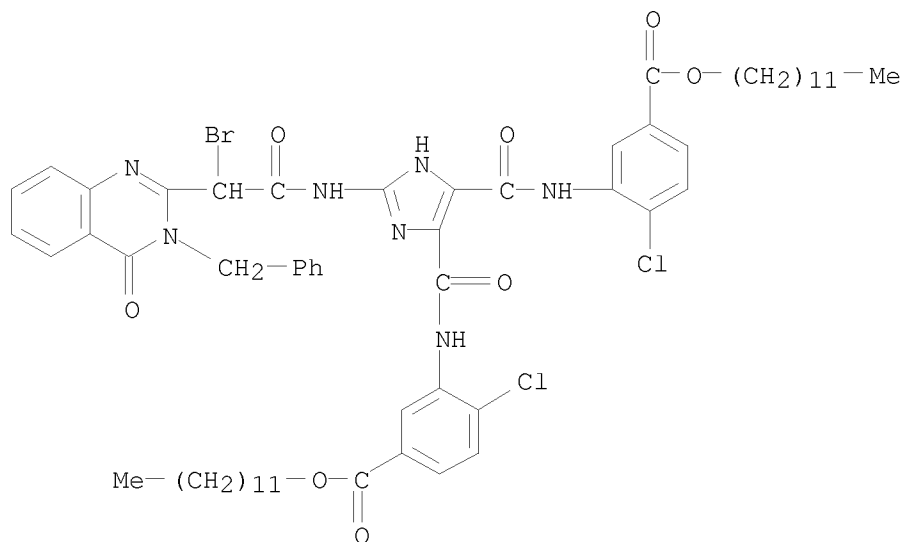
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IT 473738-63-5  
 RL: TEM (Technical or engineered material use); USES (Uses)  
 (photog. coupler for azomethine dye formation)  
 RN 473738-63-5 CAPLUS  
 CN 4H-1,2,4-Benzothiadiazine-3-acetamide,  
 $\alpha$ -(4,4-dimethyl-2,5-dioxo-1-imidazolidinyl)-N-(4,5-dimethyl-1H-  
 imidazol-2-yl)-4-dodecyl-, 1,1-dioxide (CA INDEX NAME)



IT 473738-75-9P  
 RL: PNU (Preparation, unclassified); RCT (Reactant); PREP (Preparation);  
 RACT (Reactant or reagent)  
 (preparation of photog. coupler)  
 RN 473738-75-9 CAPLUS  
 CN Benzoic acid, 3,3'-[[2-[[bromo[3,4-dihydro-4-oxo-3-(phenylmethyl)-2-  
 quinazolinyl]acetyl]amino]-1H-imidazole-4,5-diyl]bis(carbonylimino)]bis[4-  
 chloro-, didodecyl ester (9CI) (CA INDEX NAME)



L5 ANSWER 6 OF 16 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1998:682235 CAPLUS

DOCUMENT NUMBER: 129:302639

ORIGINAL REFERENCE NO.: 129:61735a, 61738a

TITLE: Preparation of imidazolylaminopropylindazolylcarbonylaminopropionate ammonioalkyl esters and related compounds as integrin  $\alpha\beta 3$  inhibitor prodrugs.

INVENTOR(S): Jadhav, Prabhakar; Batt, Douglas G.; Hussain, Munir A.; Pitts, William J.; Repta, Arnold J.

PATENT ASSIGNEE(S): Du Pont Pharmaceuticals Co., USA

SOURCE: PCT Int. Appl., 311 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9843962	A1	19981008	WO 1998-US6054	19980327 <--
W: AU, BR, CA, CN, CZ, EE, HU, IL, JP, KR, LT, LV, MX, NO, NZ, PL, RO, SG, SI, SK, UA, VN				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
AU 9867803	A	19981022	AU 1998-67803	19980327 <--
US 6214834	B1	20010410	US 1998-49305	19980327 <--
PRIORITY APPLN. INFO.:			US 1997-41759P	P 19970328
			WO 1998-US6054	W 19980327

OTHER SOURCE(S): MARPAT 129:302639

AB Title compds. [I; X1-X4 = N, C;  $\geq 2$  of X1-X4 = C; R1 = specified heterocyclalkyl; R10 = H, amino, halo, NO<sub>2</sub>, cyano, CF<sub>3</sub>, sulfonylamino, carbamoyl, (substituted) alkyl, alkoxy, alkenyl, cycloalkyl, cycloalkylalkyl, aryl, arylalkyl, etc.; R11 = H, halo, CF<sub>3</sub>, cyano, NO<sub>2</sub>, OH, amino, (substituted) alkyl, alkoxy, aryl, aralkyl, alkoxycarbonyl, alkylcarbonyl, alkylsulfonyl, alkylaminosulfonyl; W = [C(R12)2]qCONR13, CONR13[C(R12)2]q; X = CR12R14CR12R15; WX = specified piperazinylcarbonyl(alkyl); Y = COR19; R12 = H, halo, alkyl, alkenyl, alkynyl, cycloalkyl, cycloalkylalkyl, alkylcarbonyl, aryl, aralkyl; R13 = H, (substituted) alkyl, cycloalkylmethyl, aralkyl; R14 = H,

alkylthioalkyl, aralkylthioalkyl, aralkoxyalkyl, alkyl, alkoxyalkyl, hydroxyalkyl, alkenyl, alkynyl, cycloalkyl, aralkyl, heteroarylalkyl, aryl, heteroaryl, etc.; R15 = H, (substituted) alkyl, alkoxyalkyl, alkylaminoalkyl, aralkylcarbonyl, aryl, heteroaryl, heteroarylalkyl, aminosulfonyl, aminosulfonylamino, etc.; R19 = O(CH<sub>2</sub>)<sub>k</sub>N+R22R23R24 Z<sup>-</sup>; Z<sup>-</sup> = specified pharmaceutically acceptable anion; R22-R24 = H, (substituted) alkyl, cyclolalkylalkyl, aryl, aralkyl, heteroaryl, heteroarylalkyl; R22R23 = (substituted) 5-7 membered heterocyclyl; R22R23R24 = (substituted) heterobicyclyl; q = 0-2; k = 2-6], were prepared I may be administered by iontophoresis for the inhibition of cell adhesion, the treatment of angiogenic disorders, inflammation, bone degradation, cancer metastasis, diabetic retinopathy, thrombosis, restenosis, macular degeneration, and other conditions mediated by cell adhesion and/or cell migration and/or angiogenesis. Thus, title compound (II; R = CH<sub>2</sub>CH<sub>2</sub>N+Me<sub>3</sub>) showed electrophoretic mobility = 3.2 cm<sup>2</sup>/V/s at pH 4.5, vs. 1.7 cm<sup>2</sup>/V/s for II (R = Me).

IT 185561-98-2DP, esters with ammonioalkanols

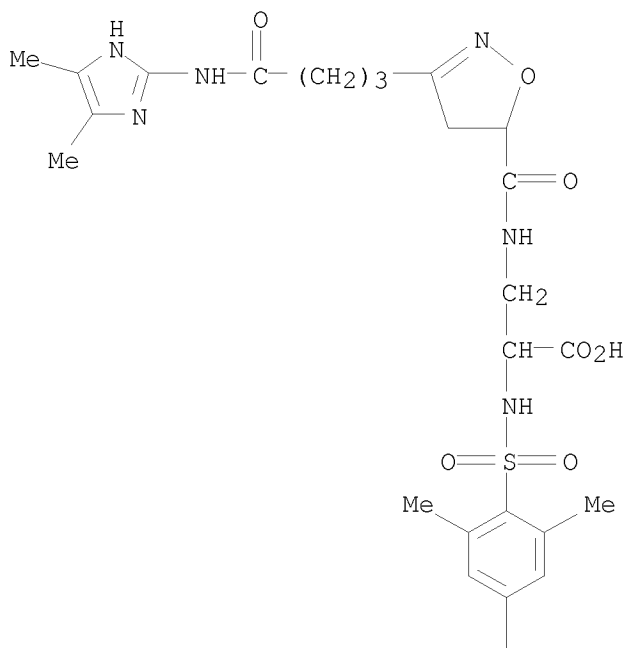
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of imidazolylaminopropylindazolylcarbonylaminopropionate ammonioalkyl esters and related compds. as integrin inhibitor prodrugs)

RN 185561-98-2 CAPLUS

CN Alanine, 3-[[[3-[4-[(4,5-dimethyl-1H-imidazol-2-yl)amino]-4-oxobutyl]-4,5-dihydro-5-isoxazolyl]carbonyl]amino]-N-[(2,4,6-trimethylphenyl)sulfonyl]-(CA INDEX NAME)

PAGE 1-A



PAGE 2-A



REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 7 OF 16 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1997:76956 CAPLUS  
DOCUMENT NUMBER: 126:89390  
ORIGINAL REFERENCE NO.: 126:17263a,17266a  
TITLE: Preparation of cyclic amides as herbicides  
INVENTOR(S): Takabe, Fumiaki; Ichinohe, Yuki; Shibayama, Atsushi;  
Yamaguchi, Mikio; Yanagisawa, Katsutada; Ogawa,  
Yasunori; Sadohara, Hideo  
PATENT ASSIGNEE(S): Kumiai Chemical Industry Co, Japan; Ihara Chemical Ind  
Co  
SOURCE: Jpn. Kokai Tokkyo Koho, 37 pp.  
CODEN: JKXXAF  
DOCUMENT TYPE: Patent  
LANGUAGE: Japanese  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 08311026	A	19961126	JP 1996-69068	19960229 <--
JP 3954127	B2	20070808		
JP 2007182456	A	20070719	JP 2007-86387	20070329
PRIORITY APPLN. INFO.:			JP 1995-81967	A 19950314
			JP 1996-69068	A3 19960229

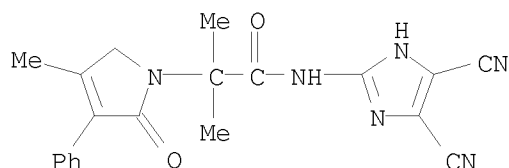
OTHER SOURCE(S): MARPAT 126:89390

AB The title compds. I [AB = NNMe, etc.; X = H, halo, etc.; m = 1 or 2; n = 1 - 3; R1 = carbamoyl with substituent, etc.] are prepared The title compound II (at 10 g) gave  $\geq 90\%$  control of Monochoria vaginalis and Scirpus juncoides.

IT 185693-68-9P  
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of cyclic amides as herbicides)

RN 185693-68-9 CAPLUS

CN 1H-Pyrrole-1-acetamide, N-(4,5-dicyano-1H-imidazol-2-yl)-2,5-dihydro- $\alpha,\alpha,4$ -trimethyl-2-oxo-3-phenyl- (CA INDEX NAME)



L5 ANSWER 8 OF 16 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1997:69816 CAPLUS  
DOCUMENT NUMBER: 126:89360  
ORIGINAL REFERENCE NO.: 126:17255a,17258a  
TITLE: Preparation of [(isoxazolinyllalkanoyl)amino]alkanoates and analogs as integrin antagonists  
INVENTOR(S): Voss, Matthew Ernst; Jadhav, Prabhakar Kondaji;  
Smallheer, Joanne Marie; Batt, Douglas Guy; Pitts,  
William John; Wityak, John  
PATENT ASSIGNEE(S): Du Pont Merck Pharmaceutical Company, USA

SOURCE: PCT Int. Appl., 331 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9637492	A1	19961128	WO 1996-US7646	19960524 <--
W: AM, AT, AU, AZ, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, HU, JP, KG, KR, KZ, LT, LU, LV, MD, MX, NO, NZ, PL, PT, RO, RU, SE, SG, SI, SK, TJ, TM, UA, VN				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
US 5710159	A	19980120	US 1996-647132	19960509 <--
CA 2221980	A1	19961128	CA 1996-2221980	19960524 <--
AU 9658762	A	19961211	AU 1996-58762	19960524 <--
ZA 9604195	A	19971124	ZA 1996-4195	19960524 <--
EP 828737	A1	19980318	EP 1996-920476	19960524 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
JP 11506436	T	19990608	JP 1996-535899	19960524 <--
PRIORITY APPLN. INFO.:			US 1995-450646	A 19950525
			US 1995-455768	A 19950531
			US 1996-647132	A 19960509
			WO 1996-US7646	W 19960524

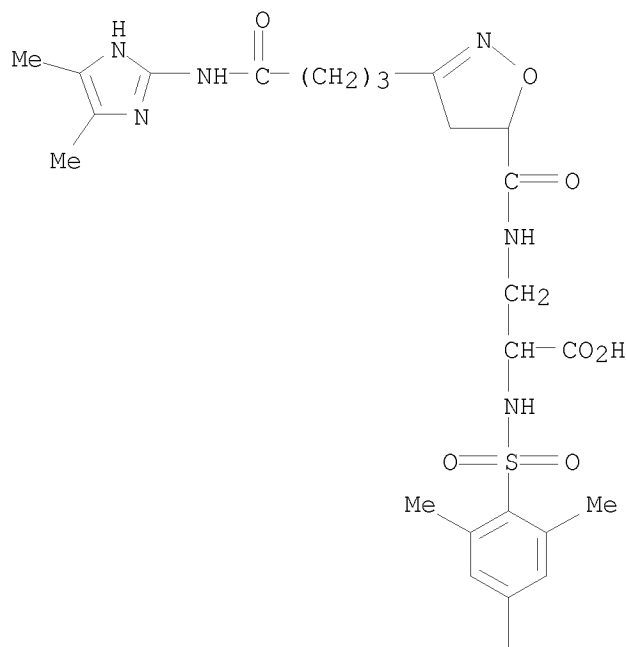
OTHER SOURCE(S): MARPAT 126:89360

AB Title compds. [(addnl.-substituted) I; R2 = Z2Z1R1; R1 = N-containing heterocyclyl; R3 = Z3ZR; R = CO2H, alkoxycarbonyl, SO3H, CONHNHSO2CF3, etc.; Z = bond (un)substituted alkylene; Z1 = bond, (O- or N-interrupted)alkylene, CO, alkanoyl(alkyl), NHCO, etc.; Z2 = bond, alkylene, phenylene, etc.; Z3 = (alkylene)carbonylimino(alkyl), etc.; dashed line = optional bond] were prepared as integrin antagonists (no data). Thus, R4(CH2)3CH:NOH (R4 = phthalimido)(preparation given) was chlorinated and the product cyclocondensed with CH2:CHCH2CO2CMe3 to give, after deprotection, tert-Bu 3-(3-aminopropyl)-2-isoxazoline-5-acetate. The latter was N-alkylated with 2-methylthio-3,4,5,6-tetrahydropyrimidine hydroiodide to give, after saponification, amidation by H2NCH2CH(NHSO2Ph)CO2Me, and saponification, title compound II.

IT 185561-98-2P  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of [(isoxazolinylalkanoyl)amino]alkanoates and analogs as integrin antagonists)

RN 185561-98-2 CAPLUS

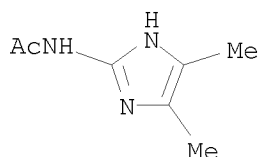
CN Alanine, 3-[[[3-[4-[(4,5-dimethyl-1H-imidazol-2-yl)amino]-4-oxobutyl]-4,5-dihydro-5-isoxazolyl]carbonyl]amino]-N-[(2,4,6-trimethylphenyl)sulfonyl]-(CA INDEX NAME)



Me

L5 ANSWER 9 OF 16 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1995:183280 CAPLUS  
 DOCUMENT NUMBER: 122:55805  
 ORIGINAL REFERENCE NO.: 122:10814h,10815a  
 TITLE: A Simple and Practical Synthesis of 2-Aminoimidazoles  
 AUTHOR(S): Little, Thomas L.; Webber, Stephen E.  
 CORPORATE SOURCE: Agouron Pharmaceuticals Inc., San Diego, CA, 92121, USA  
 SOURCE: Journal of Organic Chemistry (1994), 59(24), 7299-305  
 CODEN: JOCEAH; ISSN: 0022-3263  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 122:55805  
 AB A new and simple two-step procedure to synthesize 2-aminoimidazoles (2-AI's) from readily available materials has been developed. The cyclization reaction of  $\alpha$ -halo ketones  $\text{RCOCHR}_1\text{X}$  [ $\text{R} = \text{Me, Et, CMe}_3, \text{Ph, 4-BrC}_6\text{H}_4$ , etc.,  $\text{R}_1 = \text{H, Me, Ph}$ ,  $\text{RR}_1 = (\text{CH}_2)_3, (\text{CH}_2)_4$ ,  $\text{X} = \text{Cl, Br}$ ] and N-acetylguanidine in acetonitrile ( $\text{MeCN}$ ) at reflux, or in DMF at ambient temperature, gives 4(5)-substituted and 4,5-disubstituted N-(1H-imidazol-2-yl)acetamides I, which are then hydrolyzed to their resp. 2-AI's. In general, the purified products were isolated in good yields. We have prepared several examples and have demonstrated the usefulness of this method by its application in the total synthesis of 2-aminohistamine, an interesting histamine analog, and oroidin (II), a marine natural product isolated from various sponges.

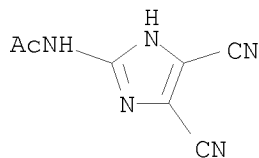
IT 40639-97-2P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (preparation of aminoimidazoles, aminohistamine, and oroidin by cyclization  
 of carbonyl with acetylguanidine)  
 RN 40639-97-2 CAPLUS  
 CN Acetamide, N-(4,5-dimethyl-1H-imidazol-2-yl)- (CA INDEX NAME)



L5 ANSWER 10 OF 16 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1978:105227 CAPLUS  
 DOCUMENT NUMBER: 88:105227  
 ORIGINAL REFERENCE NO.: 88:16505a,16508a  
 TITLE: Thiocarbonyl ylides of 1,3-diazacyclopentadiene and of  
 cyclopentadiene  
 AUTHOR(S): Gronski, Peter; Hartke, Klaus  
 CORPORATE SOURCE: Inst. Pharm. Chem., Univ. Marburg, Marburg, Fed. Rep.  
 Ger.  
 SOURCE: Chemische Berichte (1978), 111(1), 272-81  
 CODEN: CHBEAM; ISSN: 0009-2940  
 DOCUMENT TYPE: Journal  
 LANGUAGE: German  
 OTHER SOURCE(S): CASREACT 88:105227

AB R1R2NCSNR3R4 (R1-R4 = H, Me; R1 = Me, R2 = R4 = H, R3 = Me, R2-R4 = H,  
 R2R3 = CH2CH2, R4 = H, Me, R2R3 = o-C6H4, R4 = Me; R1 = R4 = H, R2R3 =  
 CH2CH2) reacted with imidazole I at room temperature to give 36-57%  
 isothiuronium salts II (Z = bond) by elimination of N2. At 0°,  
 25-94% II (Z = N:N) were isolated as labile intermediates. Analogously,  
 cyclopentadienide III (R5 = cyano, R6 = H) and N2NCSNH2 gave 8%  
 isothiuronium salt IV (R1-R4, R6 = H, R5 = cyano); III (R5 = H, R6 =  
 cyano) with R1R2NCSNR3R4 (R1 = R3 = H, R2 = R4 = Me; R1-R4 : Me; R1 = Me,  
 R2R3 = CH2CH2, R4 = H, Me; R1 = R4 = Me; R2R3 = o-C6H4) gave 1.5-75% IV  
 (R5 v H, R6 = cyano). Ylides II (Z = bond) and IV are thermally stable  
 and are betaines.

IT 65739-60-8P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 65739-60-8 CAPLUS  
 CN Acetamide, N-(4,5-dicyano-1H-imidazol-2-yl)- (CA INDEX NAME)



L5 ANSWER 11 OF 16 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1976:405638 CAPLUS

DOCUMENT NUMBER: 85:5638  
 ORIGINAL REFERENCE NO.: 85:907a,910a  
 TITLE: 2-Acylamino-4,5-di-cyanoimidazoles  
 INVENTOR(S): Segawa, Hirozo; Aida, Kazuhiko; Takagi, Toshiaki  
 PATENT ASSIGNEE(S): Kyowa Gas Chemical Industry Co., Ltd., Japan  
 SOURCE: Jpn. Kokai Tokkyo Koho, 3 pp.  
 CODEN: JKXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

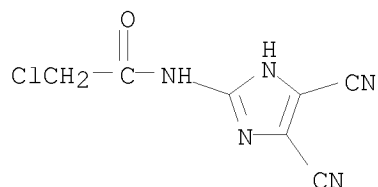
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 51004171	A	19760114	JP 1974-74630	19740629 <--
PRIORITY APPLN. INFO.:			JP 1974-74630	A 19740629

AB The title imidazoles I (R1 = C1-16 alkyl, C6-14 aryl) were prepared by reacting II with RCOCl. Thus, 3.1 g p-MeC6H4COCl in THF was refluxed with 2.6 g II and pyridine in THF 2 hr to give I (R = C6H4Me-p). Among 6 more I similarly prepared were (R given); C6H4NO2-p, CH2Cl, CMe:CH2, CH2OPh.

IT 59380-96-0P 59380-97-1P 59380-98-2P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)

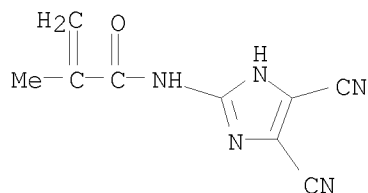
RN 59380-96-0 CAPLUS

CN Acetamide, 2-chloro-N-(4,5-dicyano-1H-imidazol-2-yl)- (CA INDEX NAME)



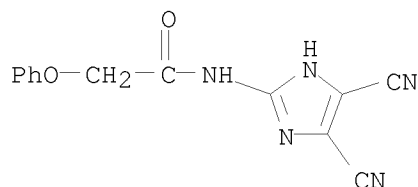
RN 59380-97-1 CAPLUS

CN 2-Propenamide, N-(4,5-dicyano-1H-imidazol-2-yl)-2-methyl- (CA INDEX NAME)



RN 59380-98-2 CAPLUS

CN Acetamide, N-(4,5-dicyano-1H-imidazol-2-yl)-2-phenoxy- (CA INDEX NAME)



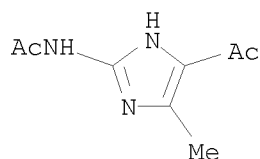
ACCESSION NUMBER: 1975:112006 CAPLUS  
 DOCUMENT NUMBER: 82:112006  
 ORIGINAL REFERENCE NO.: 82:17899a,17902a  
 TITLE: Mononuclear heterocyclic rearrangements. VI.  
 Conversion of 1,2,4-oxadiazoles into imidazoles  
 AUTHOR(S): Ruccia, M.; Vivona, N.; Cusmano, G.  
 CORPORATE SOURCE: Fac. Sci., Univ. Palermo, Palermo, Italy  
 SOURCE: Tetrahedron (1974), 30(21), 3859-64  
 CODEN: TETRAB; ISSN: 0040-4020  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 82:112006

AB Condensation of aminooxadiazoles with  $\beta$ -oxo ketones or esters gave  $\beta$ -enamino ketones, which with NaOEt in DMF rearranged to imidazole derivs. E.g., I with (MeCO)<sub>2</sub>CH<sub>2</sub> gave II, which with NaOEt in DMF gave III. Condensation of I with PhCOCH<sub>2</sub>CO<sub>2</sub>Et gave IV and V. V was in solution equilibrium with its tautomer VI.

IT 40483-42-9P 40483-44-1P 55729-98-1P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)

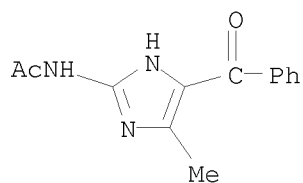
RN 40483-42-9 CAPLUS

CN Acetamide, N-(4-acetyl-5-methyl-1H-imidazol-2-yl)- (9CI) (CA INDEX NAME)



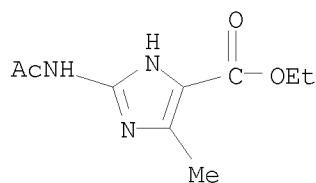
RN 40483-44-1 CAPLUS

CN Acetamide, N-(4-benzoyl-5-methyl-1H-imidazol-2-yl)- (9CI) (CA INDEX NAME)

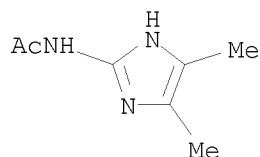


RN 55729-98-1 CAPLUS

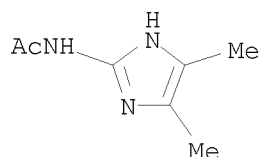
CN 1H-Imidazole-4-carboxylic acid, 2-(acetylamino)-5-methyl-, ethyl ester  
 (9CI) (CA INDEX NAME)



ACCESSION NUMBER: 1973:405297 CAPLUS  
 DOCUMENT NUMBER: 79:5297  
 ORIGINAL REFERENCE NO.: 79:898h,899a  
 TITLE: Condensations with N,N'-hydrazinodicarboxamidine. 12.  
 Proof of the 2-aminoimidazole structure by ring  
 synthesis from cyanamide  
 AUTHOR(S): Kreutzberger, A.; Schuecker, R.  
 CORPORATE SOURCE: Inst. Pharm. Chem., Westfael. Wilhelms-Univ.,  
 Muenster, Fed. Rep. Ger.  
 SOURCE: Archiv der Pharmazie (Weinheim, Germany) (1973  
 ), 306(3), 169-73  
 CODEN: ARPMAS; ISSN: 0365-6233  
 DOCUMENT TYPE: Journal  
 LANGUAGE: German  
 AB The structure of the 2-aminoimidazoles [I, R = R1 = Me or RR1 = (CH2)4]  
 formed by reduction of the corresponding 2,2'-azoimidazoles was supported by  
 their synthesis from H2NCHR1COR and H2NCN.  
 IT 40639-97-2P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 40639-97-2 CAPLUS  
 CN Acetamide, N-(4,5-dimethyl-1H-imidazol-2-yl)- (CA INDEX NAME)



L5 ANSWER 14 OF 16 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1973:124496 CAPLUS  
 DOCUMENT NUMBER: 78:124496  
 ORIGINAL REFERENCE NO.: 78:20003a,20006a  
 TITLE: Condensations with hydrazine-N,N'-dicarboxamidines.  
 11. 2-Aminoimidazoles by reduction of  
 2,2'-azoimidazoles  
 AUTHOR(S): Kreutzberger, A.; Schuecker, R.  
 CORPORATE SOURCE: Inst. Pharm. Chem., Westfael. Wilhelms-Univ.,  
 Muenster, Fed. Rep. Ger.  
 SOURCE: Archiv der Pharmazie (Weinheim, Germany) (1973  
 ), 306(2), 139-45  
 CODEN: ARPMAS; ISSN: 0365-6233  
 DOCUMENT TYPE: Journal  
 LANGUAGE: German  
 AB The aminoimidazoles XNH2 (R = H or Me) and YNH2 were obtained by reduction of  
 XN:NX or YN:Ny, resp., and were characterized by conversion into acyl  
 derivs.  
 IT 40639-97-2P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 RN 40639-97-2 CAPLUS  
 CN Acetamide, N-(4,5-dimethyl-1H-imidazol-2-yl)- (CA INDEX NAME)



L5 ANSWER 15 OF 16 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1973:97567 CAPLUS

DOCUMENT NUMBER: 78:97567

ORIGINAL REFERENCE NO.: 78:15659a,15662a

TITLE: Mononuclear heterocyclic rearrangements. V.  
1,2,4-Oxadiazoles to imidazoles

AUTHOR(S): Ruccia, Michele; Vivona, Nicolo; Cusmano, Giuseppe

CORPORATE SOURCE: Fac. Sci., Univ. Palermo, Palermo, Italy

SOURCE: Tetrahedron Letters (1972), (49), 4959-60

CODEN: TELEAY; ISSN: 0040-4039

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 78:97567

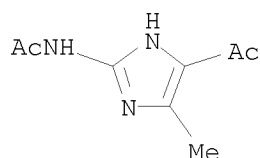
AB Condensing 3-amino-5-methyl-1,2,4-oxadiazole or the 5-Ph analog with MeCOCH<sub>2</sub>COMe or PhCOCH<sub>2</sub>COMe in refluxing PhMe containing p-MeC<sub>6</sub>H<sub>4</sub>SO<sub>3</sub>H for 8-10 hr gave the oxadiazole enamino ketones (I; R, R<sub>1</sub> = Me, Ph). Rearrangement of I with 1 equivalent NaOEt in DMF at 110° for 3 hr gave 60-80% of the corresponding imidazoles (II). Acid hydrolysis of II gave 2-aminoimidazoles.

IT 40483-42-9P 40483-44-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and acid hydrolysis of)

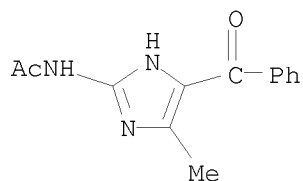
RN 40483-42-9 CAPLUS

CN Acetamide, N-(4-acetyl-5-methyl-1H-imidazol-2-yl)- (9CI) (CA INDEX NAME)



RN 40483-44-1 CAPLUS

CN Acetamide, N-(4-benzoyl-5-methyl-1H-imidazol-2-yl)- (9CI) (CA INDEX NAME)



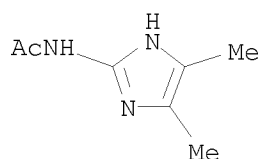
L5 ANSWER 16 OF 16 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1926:1672 CAPLUS

DOCUMENT NUMBER: 20:1672

ORIGINAL REFERENCE NO.: 20:193g-i

TITLE: 2-Amino-4,5-dimethylglyoxaline  
 AUTHOR(S): Burtles, Richard; Pyman, F. L.  
 SOURCE: Journal of the Chemical Society, Transactions ( 1925), 127, 2012-8  
 CODEN: JCHTA3; ISSN: 0368-1645  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Unavailable  
 AB 2-p-Bromobenzeneazo-4,5-dimethylglyoxaline, light brown, m. 213-4° (all m. ps. are corrected); it seems to cause irritation of the skin and swelling of the eyelids; HCl salt, orange-yellow, decomp. 135°. Reduction by Sn and HCl gives 69% of 2-amino-4,5-dimethylglyoxaline-HCl, m. 389°; carbonate, with 1H2O, m. 144°; picrate, yellow, m. 245°. The amine reacts sluggishly with HNO2 in dilute or concentrated HCl or 25% AcOH, giving no crystalline products, but the solns. give deep colors on treatment with NaOH. It gives deeply colored solns. with Na2Fe(CN)6NO and aqueous NaOH or with AmNO2 and EtONa in EtOH. Ac derivative, m. 270°; after treating with HCl and NaNO2, it gives no color with β-C10H7ONa; it instantly decolorizes aqueous KMnO4. The NH2 derivative does not give a benzylidene derivative 2-p-Bromobenzeneazo-4(5)-methylglyoxaline (I), yellow, m. 225-6°. 5(4)-p-Bromobenzeneazo derivative, brown, m. 238°; HCl salt, yellow needles or yellow-red prisms, m. 188°. The yield of these 2 compds. is about 47 and 12%. The constitution of I was established by its reduction by Zn and AcOH to alacreatinine; this is also obtained with SnCl2 and HCl, together with about 10% of the 2-amino derivative, analyzed as the picrate, brownish yellow, m. 186-7°.  
 IT 40639-97-2P, Acetamide, N-(4,5-dimethyl-2-imidazolyl)-  
 RL: PREP (Preparation)  
 (preparation of)  
 RN 40639-97-2 CAPLUS  
 CN Acetamide, N-(4,5-dimethyl-1H-imidazol-2-yl)- (CA INDEX NAME)



=>

=> ....Testing the current file.... screen

THIS COMMAND NOT AVAILABLE IN THE CURRENT FILE

Please change to a suitable file and repeat your upload

Some commands only work in certain files. For example, the EXPAND command can only be used to look at the index in a file which has an index. Enter "HELP COMMANDS" at an arrow prompt (=>) for a list of commands which can be used in this file.

=> file reg

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	97.00	275.57

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION

CA SUBSCRIBER PRICE -12.80 -12.80

FILE 'REGISTRY' ENTERED AT 11:40:27 ON 27 OCT 2008  
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STRUCTURE FILE UPDATES: 24 OCT 2008 HIGHEST RN 1065816-63-8  
DICTIONARY FILE UPDATES: 24 OCT 2008 HIGHEST RN 1065816-63-8

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TSCA INFORMATION NOW CURRENT THROUGH July 5, 2008.

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experimental property data in the original document. For information  
on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=> ....Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end

=>

Uploading C:\Program Files\STNEXP\Queries\10564010 str 3.str

L6 STRUCTURE UPLOADED

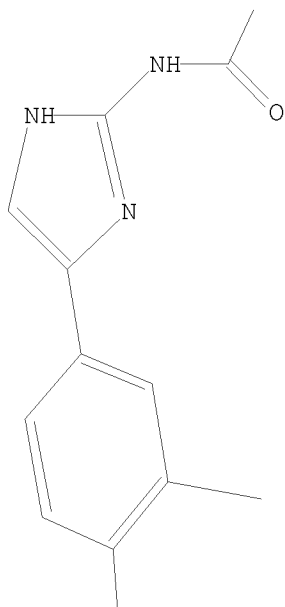
=> que L6

L7 QUE L6

=> d ;7

L7 HAS NO ANSWERS

L6 STR



Structure attributes must be viewed using STN Express query preparation.  
 L7 QUE ABB=ON PLU=ON L6

7 IS NOT A RECOGNIZED COMMAND

The previous command name entered was not recognized by the system.  
 For a list of commands available to you in the current file, enter  
 "HELP COMMANDS" at an arrow prompt (=>).

=> s l7 sss full

FULL SEARCH INITIATED 11:40:51 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 2382 TO ITERATE

100.0% PROCESSED 2382 ITERATIONS

1 ANSWERS

SEARCH TIME: 00.00.01

L8 1 SEA SSS FUL L6

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

178.36

453.93

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

0.00

-12.80

FILE 'CAPLUS' ENTERED AT 11:40:57 ON 27 OCT 2008

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FILE COVERS 1907 - 27 Oct 2008 VOL 149 ISS 18  
FILE LAST UPDATED: 26 Oct 2008 (20081026/ED)

Caplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2008.

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

<http://www.cas.org/legal/infopolicy.html>

=> s l8

L9 0 L8

=> d his

(FILE 'HOME' ENTERED AT 11:30:00 ON 27 OCT 2008)

FILE 'REGISTRY' ENTERED AT 11:30:38 ON 27 OCT 2008

L1 STRUCTURE UPLOADED

L2 QUE L1

L3 22 S L2 SSS FULL

FILE 'CAPLUS' ENTERED AT 11:31:05 ON 27 OCT 2008

L4 22 S L3

L5 16 S L4 AND PY<=2004

FILE 'REGISTRY' ENTERED AT 11:40:27 ON 27 OCT 2008

L6 STRUCTURE UPLOADED

L7 QUE L6

L8 1 S L7 SSS FULL

FILE 'CAPLUS' ENTERED AT 11:40:57 ON 27 OCT 2008

L9 0 S L8

=> s l7

SEARCH PROFILE NOT SUPPORTED FOR AUTOMATED SEARCH AND CROSSOVER

The search profile contains L-numbers or saved item names that include chemical substance terms, chemical structures, or structure screen sets. If you are in a single file environment using the CA file (CA, HCA, ZCA, CAPLUS, HCAPLUS, ZCAPLUS), enter HELP FIRST at an arrow prompt (=) for information about the REGISTRY automated search and crossover feature. REGISTRY supports the following search profiles:

Example 1:

=> ACT SCRSTR/Q

L3 STR

L4 SCR 2127

L5 QUE L3 NOT L4

These searches are supported:

S L5/REG

S SCRSTR/Q/REG

S (L3 NOT L4)/REG

These searches are not supported:

S L5  
S SCRSTR/Q

Example 2:

=> ACT SCRSTR2/Q  
L6 STR  
L7 SCR 2127  
L8 QUE L6  
L9 QUE L7  
L10 QUE L8 NOT L9

This search is supported:

S (L6 NOT L7)/REG

These searches are not supported:

S L10  
S L10/REG  
S SCRSTR2/Q  
S SCRSTR2/Q/REG  
S L8 NOT L9  
S (L8 NOT L9)/REG

=> s 18  
L10 0 L8

=> file reg		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	0.96	454.89
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-12.80

FILE 'REGISTRY' ENTERED AT 11:42:15 ON 27 OCT 2008  
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STRUCTURE FILE UPDATES: 24 OCT 2008 HIGHEST RN 1065816-63-8  
DICTIONARY FILE UPDATES: 24 OCT 2008 HIGHEST RN 1065816-63-8

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TSCA INFORMATION NOW CURRENT THROUGH July 5, 2008.

Please note that search-term pricing does apply when  
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REGISTRY includes numerically searchable data for experimental and  
predicted properties as well as tags indicating availability of  
experimental property data in the original document. For information  
on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=> ....Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end

=>

Uploading C:\Program Files\STNEXP\Queries\10564010 str 4.str

L11 STRUCTURE UPLOADED

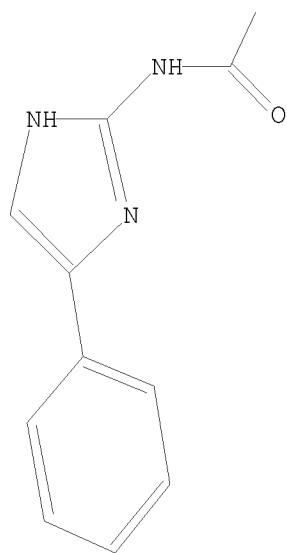
=> que L11

L12 QUE L11

=> d l12

L12 HAS NO ANSWERS

L11 STR



Structure attributes must be viewed using STN Express query preparation.

L12 QUE ABB=ON PLU=ON L11

=> s l12 sss full

FULL SEARCH INITIATED 11:42:49 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 5244 TO ITERATE

100.0% PROCESSED 5244 ITERATIONS

126 ANSWERS

SEARCH TIME: 00.00.01

L13 126 SEA SSS FUL L11

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

178.36

633.25

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

0.00

-12.80

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FILE COVERS 1907 - 27 Oct 2008 VOL 149 ISS 18  
FILE LAST UPDATED: 26 Oct 2008 (20081026/ED)

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<http://www.cas.org/legal/infopolicy.html>

=> s l13

L14 44 L13

=> s l14 and py<=2004

25113423 PY<=2004

L15 24 L14 AND PY<=2004

=> s l15 and 5-hydroxytryptamine

6834776 5

20870 HYDROXYTRYPTAMINE

71 HYDROXYTRYPTAMINES

20895 HYDROXYTRYPTAMINE

(HYDROXYTRYPTAMINE OR HYDROXYTRYPTAMINES)

20023 5-HYDROXYTRYPTAMINE

(5(W)HYDROXYTRYPTAMINE)

L16 0 L15 AND 5-HYDROXYTRYPTAMINE

=> s l15 and 5HT

3174 5HT

L17 0 L15 AND 5HT

=> s l15 1-24 ibib ab hitstr

MISSING OPERATOR L15 1-24

The search profile that was entered contains terms or nested terms that are not separated by a logical operator.

=> s l15 1-24 ibib ab hitstr

MISSING OPERATOR L15 1-24

The search profile that was entered contains terms or nested terms that are not separated by a logical operator.

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

FULL ESTIMATED COST	ENTRY 9.92	SESSION 643.17
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-12.80

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FILE COVERS 1907 - 27 Oct 2008 VOL 149 ISS 18  
 FILE LAST UPDATED: 26 Oct 2008 (20081026/ED)

Caplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2008.

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

<http://www.cas.org/legal/infopolicy.html>

=> d his

(FILE 'HOME' ENTERED AT 11:30:00 ON 27 OCT 2008)

FILE 'REGISTRY' ENTERED AT 11:30:38 ON 27 OCT 2008

L1 STRUCTURE UPLOADED  
 L2 QUE L1  
 L3 22 S L2 SSS FULL

FILE 'CAPLUS' ENTERED AT 11:31:05 ON 27 OCT 2008

L4 22 S L3  
 L5 16 S L4 AND PY<=2004

FILE 'REGISTRY' ENTERED AT 11:40:27 ON 27 OCT 2008

L6 STRUCTURE UPLOADED  
 L7 QUE L6  
 L8 1 S L7 SSS FULL

FILE 'CAPLUS' ENTERED AT 11:40:57 ON 27 OCT 2008

L9 0 S L8  
 L10 0 S L8

FILE 'REGISTRY' ENTERED AT 11:42:15 ON 27 OCT 2008

L11 STRUCTURE UPLOADED  
 L12 QUE L11  
 L13 126 S L12 SSS FULL

FILE 'CAPLUS' ENTERED AT 11:42:56 ON 27 OCT 2008

L14 44 S L13  
 L15 24 S L14 AND PY<=2004  
 L16 0 S L15 AND 5-HYDROXYTRYPTAMINE  
 L17 0 S L15 AND 5HT

FILE 'CAPLUS' ENTERED AT 11:44:31 ON 27 OCT 2008

=> s l15 1-24 ibib ab hitstr  
 MISSING OPERATOR L15 1-24  
 The search profile that was entered contains terms or  
 nested terms that are not separated by a logical operator.

=> d l15 1-24 ibib ab hitstr

L15 ANSWER 1 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:80450 CAPLUS  
 DOCUMENT NUMBER: 140:145835  
 TITLE: Preparation of dibenzofused  
 bicyclo[2.2.2]octane-derived amides as modulators of  
 the glucocorticoid receptor

INVENTOR(S): Vaccaro, Wayne; Yang, Bingwei Vera; Kim, Soong-hoon;  
 Huynh, Tram; Tortolani, David R.; Leavitt, Kenneth J.;  
 Li, Wenying; Doweyko, Arthur M.; Chen, Xiao-tao;  
 Doweyko, Lidia

PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA; et al.  
 SOURCE: PCT Int. Appl., 265 pp.  
 CODEN: PIXXD2

DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004009017	A2	20040129	WO 2003-US22300	20030717 <--
WO 2004009017	A3	20040708		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
AU 2003251970	A1	20040209	AU 2003-251970	20030717 <--
US 20040132758	A1	20040708	US 2003-621909	20030717 <--
US 6995181	B2	20060207		
EP 1534273	A2	20050601	EP 2003-765638	20030717
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK			
JP 2006508042	T	20060309	JP 2004-523482	20030717
NO 2005000074	A	20050309	NO 2005-74	20050106
US 20050171136	A1	20050804	US 2005-85347	20050321
PRIORITY APPLN. INFO.:			US 2002-396877P	P 20020718
			US 2003-621909	A1 20030717
			WO 2003-US22300	W 20030717

OTHER SOURCE(S): MARPAT 140:145835

AB Title compds. I [R-R4 = H, alk(en/yn)yl, alkoxy, aryl, etc.; Z =

carboxamido, alkylamino, etc.] are prepared For instance, 2-amino-4,5-dimethylthiazole is coupled to the acid derived from the cycloaddn. of methacrylic acid and anthracene (CH<sub>3</sub>CN, EDCI, Et<sub>3</sub>N, HOAt, 18 h) to give II. I are glucocorticoid receptor modulators which are useful in treating diseases requiring glucocorticoid receptor agonist or antagonist therapy such as obesity, diabetes, inflammatory and immune disorders.

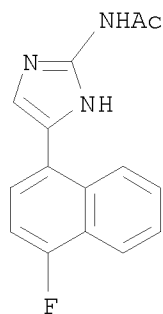
IT 650626-13-4 650626-17-8

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of dibenzofused bicyclo[2.2.2]octane-derived amides as modulators of glucocorticoid receptor)

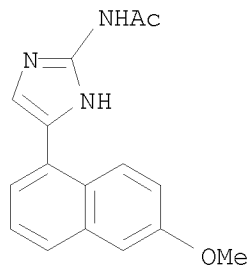
RN 650626-13-4 CAPLUS

CN Acetamide, N-[5-(4-fluoro-1-naphthalenyl)-1H-imidazol-2-yl]- (CA INDEX NAME)



RN 650626-17-8 CAPLUS

CN Acetamide, N-[5-(6-methoxy-1-naphthalenyl)-1H-imidazol-2-yl]- (CA INDEX NAME)



L15 ANSWER 2 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:80449 CAPLUS

DOCUMENT NUMBER: 140:157927

TITLE: Homology modeling of nuclear hormone receptor Site II and design of Site II ligands

INVENTOR(S): Dowejko, Arthur; Nadler, Steven G.

PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA

SOURCE: PCT Int. Appl., 276 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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WO 2004009016      A2      20040129      WO 2003-US22299      20030717 <--
W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
    CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
    GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
    LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM,
    PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN,
    TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW:  GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
    KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
    FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,
    BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
EP 1575502          A2      20050921      EP 2003-765637      20030717
EP 1575502          A3      20051123
R:   AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
    IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
US 20060223110      A1      20061005      US 2003-621807      20030717
PRIORITY APPLN. INFO.:
                                US 2002-396907P      P      20020718
                                WO 2003-US22299      W      20030717

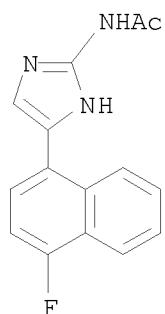
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AB A binding site in nuclear hormone receptors is described and its structural coordinates are provided. The invention provides machine-readable data storage media comprising structure coordinates of Site II and computer systems comprising the machine-readable data storage media. The invention provides methods used in the design and identification of ligands of Site II and of modulators of nuclear hormone receptors. The invention provides ligands of Site II, modulators of NHRs, pharmaceutical compns. comprising modulators of NHRs, methods of modulating NHRs, and methods of treating diseases by administering modulators of an NHR. Also provided are methods of designing mutants, mutant NHRs, Site II binding assays, and models of Site II.

IT 650626-13-4P 650626-17-8P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (homol. modeling of nuclear hormone receptor Site II in ligand binding domain and design of Site II ligands)

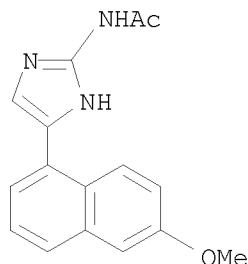
RN 650626-13-4 CAPLUS

CN Acetamide, N-[5-(4-fluoro-1-naphthalenyl)-1H-imidazol-2-yl]- (CA INDEX NAME)



RN 650626-17-8 CAPLUS

CN Acetamide, N-[5-(6-methoxy-1-naphthalenyl)-1H-imidazol-2-yl]- (CA INDEX NAME)



L15 ANSWER 3 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:41450 CAPLUS

DOCUMENT NUMBER: 140:87668

TITLE: Therapeutic imidazole compounds, and human cellular proteins casein kinase I  $\alpha$ ,  $\delta$ , and  $\epsilon$  as targets for medical intervention against hepatitis C virus infection

INVENTOR(S): Salassidis, Konstadinos; Kurtenbach, Alexander; Daub, Henrik; Obert, Sabine

PATENT ASSIGNEE(S): Axxima Pharmaceuticals A.-G., Germany; Greff, Zoltan; Keri, Gyoergy; Oerfi, Laszlo; Waczek, Frigyes

SOURCE: PCT Int. Appl., 89 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

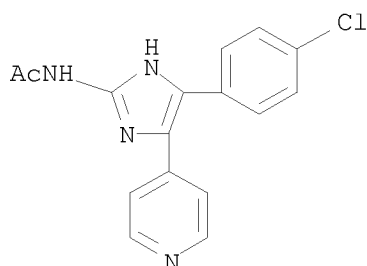
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004005264	A2	20040115	WO 2003-EP7286	20030707 <--
WO 2004005264	A3	20040304		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
AU 2003249977	A1	20040123	AU 2003-249977	20030707 <--
EP 1532118	A2	20050525	EP 2003-762649	20030707
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK			
US 20050203155	A1	20050915	US 2005-30538	20050105
PRIORITY APPLN. INFO.:			EP 2002-15096	A 20020705
			WO 2003-EP7286	W 20030707

OTHER SOURCE(S): MARPAT 140:87668

AB The invention describes imidazole compds. which are particularly useful against Hepatitis C Virus infections and diseases associated therewith. Furthermore, the invention relates to the human cellular proteins casein kinase I  $\alpha$ ,  $\delta$ , and  $\epsilon$  as targets for medical intervention against Hepatitis C Virus (HCV) infections and diseases. In addition, the invention refers to a method for the identification of compds. which are useful for the prophylaxis and/or treatment of infections and diseases caused by Hepatitis C Virus, methods for treating Hepatitis C Virus infections and diseases, as well as pharmaceutical compns. useful

for the prophylaxis and/or treatment of Hepatitis C Virus infections and diseases. Moreover, the invention discloses antibodies, oligonucleotides, and specific compds. which are effective for the detection, prophylaxis and/or treatment of infections and diseases caused by Hepatitis C Virus. In addition, the invention describes solid supports useful for the identification of compds. suitable for preventing and/or treating infections and diseases caused by Hepatitis C Virus.

IT 643750-56-5  
 RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
 (therapeutic imidazole compds., and human cellular casein kinase I  $\alpha$ ,  $\delta$ , and  $\epsilon$  as targets for medical intervention against hepatitis C virus infection)  
 RN 643750-56-5 CAPLUS  
 CN Acetamide, N-[4-(4-chlorophenyl)-5-(4-pyridinyl)-1H-imidazol-2-yl]- (CA INDEX NAME)



L15 ANSWER 4 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2003:511143 CAPLUS

DOCUMENT NUMBER: 139:85387

TITLE: Preparation of heterocyclic substituted phenylsulfonamides as broad-spectrum HIV protease inhibitors

INVENTOR(S): Vendeville, Sandrine Marie Helene; Verschueren, Wim Gaston; Tahri, Abdellah; Moors, Samuel Leo Christiaan; Erra Sola, Montserrat

PATENT ASSIGNEE(S): Tibotec Pharmaceuticals Ltd., Ire.

SOURCE: PCT Int. Appl., 74 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003053435	A1	20030703	WO 2002-EP14839	20021220 <--
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
CA 2470964	A1	20030703	CA 2002-2470964	20021220 <--

AU 2002361235	A1	20030709	AU 2002-361235	20021220 <--
AU 2002361235	B2	20080724		
EP 1463502	A1	20041006	EP 2002-796754	20021220 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
BR 2002015260	A	20041207	BR 2002-15260	20021220 <--
JP 2005513102	T	20050512	JP 2003-554192	20021220
CN 1620292	A	20050525	CN 2002-828166	20021220
HU 2005000164	A2	20050530	HU 2005-164	20021220
MX 2004PA06201	A	20041206	MX 2004-PA6201	20040621 <--
NZ 533665	A	20051028	NZ 2004-533665	20040621
IN 2004DN01777	A	20050401	IN 2004-DN1777	20040622
NO 2004003114	A	20040920	NO 2004-3114	20040720 <--
ZA 2004005784	A	20050831	ZA 2004-5784	20040720
US 20050222215	A1	20051006	US 2005-499221	20050412

PRIORITY APPLN. INFO.:

EP 2001-205115	A	20011221
WO 2002-EP14839	W	20021220

OTHER SOURCE(S): MARPAT 139:85387

AB R1LN(R2)CHR3CH(OH)CH2N(R4)SO2C6H4R5 [R1 = H, alkyl, alkenyl, aralkyl, cycloalkyl, cycloalkylalkyl, aryl, heterocyclic, heterocyclylalkyl, (un)substituted CH2CH2NH2; L = CO, O2C, (un)substituted NHCO, oxaalkylcarbonyl, aminoalkylcarbonyl, SO2, O3S, (un)substituted NHSO2; R2 = H, alkyl; R3 = alkyl, aryl, cycloalkyl, cycloalkylalkyl, aralkyl; R4 = H, (un)substituted CO2H, CONH2, cycloalkyl, alkenyl, alkynyl, alkyl; R5 = (un)substituted heteroaryl] were prepared for use as broad-spectrum HIV protease inhibitors. Thus, (1S,2R)-Me3CO2CNHCH(CH2Ph)CH(OH)CH2NHCH2CHMe2 was treated with 4-NCC6H4SO2Cl to give (1S,2R)-Me3CO2CNHCH(CH2Ph)CH(OH)CH2N(CH2CHMe2)SO2C6H4CN-4 which was deblocked and treated with the hexahydrofurofuranyloxycarbonyloxypyrrolidinedione to give the carbamate I [R6 = CN]. Treatment of I [R6 = CN] with NH2OH.HCl gave I [R6 = C(NH2):NOH] which was cyclized with 2-furoyl chloride to give I [R6 = 5-(2-furyl)-1,2,4-oxadiazol-3-yl] which had pEC50 = 8.4 for inhibition of HIV-1.

IT 553644-43-2P

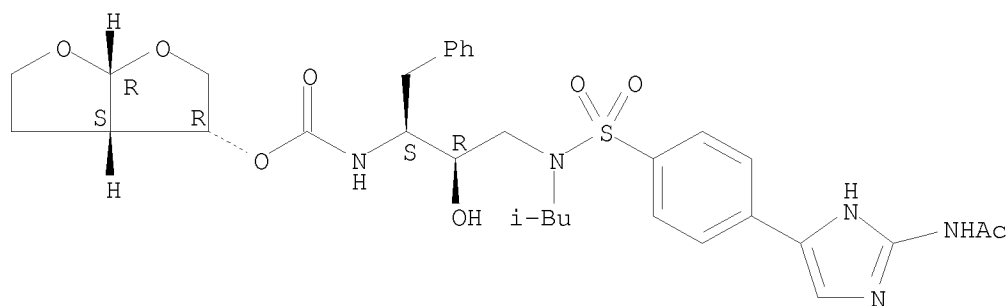
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of heterocyclic substituted phenylsulfonamides as broad-spectrum HIV protease inhibitors)

RN 553644-43-2 CAPLUS

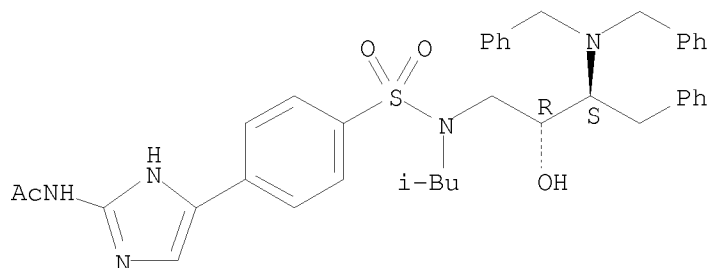
CN Carbamic acid, [(1S,2R)-3-[[[4-[2-(acetylamino)-1H-imidazol-4-yl]phenyl]sulfonyl](2-methylpropyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-, (3R,3aS,6aR)-hexahydrofuro[2,3-b]furan-3-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



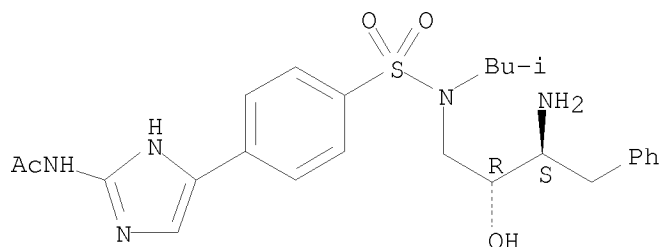
IT 553645-06-0P 553645-07-1P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (preparation of heterocyclic substituted phenylsulfonamides as  
 broad-spectrum HIV protease inhibitors)  
 RN 553645-06-0 CAPLUS  
 CN Acetamide, N-[5-[4-[[[(2R,3S)-3-[bis(phenylmethyl)amino]-2-hydroxy-4-  
 phenylbutyl](2-methylpropyl)amino]sulfonyl]phenyl]-1H-imidazol-2-yl]- (CA  
 INDEX NAME)

Absolute stereochemistry.



RN 553645-07-1 CAPLUS  
 CN Acetamide, N-[5-[4-[[[(2R,3S)-3-amino-2-hydroxy-4-phenylbutyl](2-  
 methylpropyl)amino]sulfonyl]phenyl]-1H-imidazol-2-yl]- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 5 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2003:58069 CAPLUS  
 DOCUMENT NUMBER: 138:122639  
 TITLE: Preparation of thiazols and related compounds as  
 telomerase inhibitors  
 INVENTOR(S): Priepke, Henning; Kauffmann-Hefner, Iris; Hael, Norbert; Damm, Klaus; Schnapp, Andreas  
 PATENT ASSIGNEE(S): Boehringer Ingelheim Pharma K.-G., Germany  
 SOURCE: PCT Int. Appl., 88 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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WO 2003006443 A2 20030123 WO 2002-EP7558 20020706 <--  
 WO 2003006443 A3 20030501  
 W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,  
 CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,  
 GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,  
 LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,  
 PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,  
 UA, UG, US, UZ, VN, YU, ZA, ZM, ZW  
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,  
 KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,  
 FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF,  
 CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG  
 DE 10133665 A1 20030130 DE 2001-10133665 20010711 <--  
 AU 2002328323 A1 20030129 AU 2002-328323 20020706 <--  
 US 20030055263 A1 20030320 US 2002-192456 20020710 <--  
 PRIORITY APPLN. INFO.: DE 2001-10133665 A 20010711  
 US 2001-307449P P 20010724  
 WO 2002-EP7558 W 20020706

OTHER SOURCE(S): MARPAT 138:122639

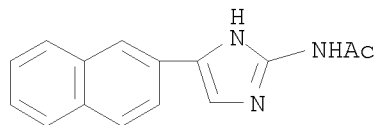
AB Title compds. R1-A-B-R2 (I) [ R1 = (un)substituted Ph, phenylalkyl, phenylalkenyl, etc.; A = (un)substituted phenylalkyl; B = HN, NHCO, CONH, etc.; R2 = CO2, (un)substituted cycloalkyl, cycloalkenyl, etc.] and their pharmaceutically acceptable salts were prepared For example, coupling of thiazol II and phthalic anhydride afforded claimed benzoic acid III in 30% yield. In telomerase inhibition studies, 3-specific examples of I exhibited IC50 values ranging from < 1 - < 5  $\mu$ M, e.g., IC50 value of compound III was < 5  $\mu$ M. Compds. I are claimed useful as telomerase inhibitors.

IT 160072-53-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (intermediate; preparation of thiazols and related compds. as telomerase inhibitors)

RN 160072-53-7 CAPLUS

CN Acetamide, N-[5-(2-naphthalenyl)-1H-imidazol-2-yl]- (CA INDEX NAME)



L15 ANSWER 6 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2002:855867 CAPLUS

DOCUMENT NUMBER: 139:214346

TITLE: Product class 3: imidazoles

AUTHOR(S): Grimmett, M. R.

CORPORATE SOURCE: Organic Chemistry, Dept. of Chemistry, University of Otago, Dunedin, N. Z.

SOURCE: Science of Synthesis (2002), 12, 325-528  
 CODEN: SSCYJ9

PUBLISHER: Georg Thieme Verlag

DOCUMENT TYPE: Journal; General Review

LANGUAGE: English

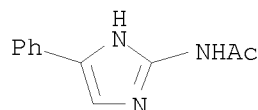
AB A review. Methods for preparing imidazoles are reviewed including cyclization, ring transformations, aromatization and modification of substituents on existing imidazoles.

IT 160041-64-5P 160072-51-5P 160072-52-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(preparation of imidazoles via cyclization, ring transformation,  
aromatization and substituent modifications)

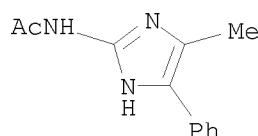
RN 160041-64-5 CAPLUS

CN Acetamide, N-(5-phenyl-1H-imidazol-2-yl)- (CA INDEX NAME)



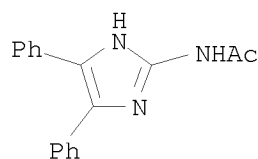
RN 160072-51-5 CAPLUS

CN Acetamide, N-(4-methyl-5-phenyl-1H-imidazol-2-yl)- (CA INDEX NAME)



RN 160072-52-6 CAPLUS

CN Acetamide, N-(4,5-diphenyl-1H-imidazol-2-yl)- (CA INDEX NAME)



REFERENCE COUNT: 823 THERE ARE 823 CITED REFERENCES AVAILABLE FOR  
THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE  
FORMAT

L15 ANSWER 7 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2002:773670 CAPLUS

DOCUMENT NUMBER: 137:279200

TITLE: Preparation of novel benzotriazoles as  
anti-inflammatory compounds

INVENTOR(S): Dombroski, Mark Anthony; Laird, Ellen Ruth; Letavic,  
Michael Anthony; McClure, Kim Francis

PATENT ASSIGNEE(S): Pfizer Products Inc., USA

SOURCE: Eur. Pat. Appl., 69 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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EP 1247810	A1	20021009	EP 2002-252153	20020326 <--
EP 1247810	B1	20050907		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,				

IE, SI, LT, LV, FI, RO, MK, CY, AL, TR

AT 304009	T	20050915	AT 2002-252153	20020326
ES 2247271	T3	20060301	ES 2002-252153	20020326
CA 2379903	A1	20021004	CA 2002-2379903	20020402 <--
CA 2379903	C	20060801		
JP 2002308872	A	20021023	JP 2002-102969	20020404 <--
JP 3832646	B2	20061011		
US 20030078432	A1	20030424	US 2002-115952	20020404 <--
US 6664395	B2	20031216		
BR 2002001087	A	20030527	BR 2002-1087	20020404 <--
MX 2002PA03454	A	20040716	MX 2002-PA3454	20020404 <--
PRIORITY APPLN. INFO.:			US 2001-281331P	P 20010404

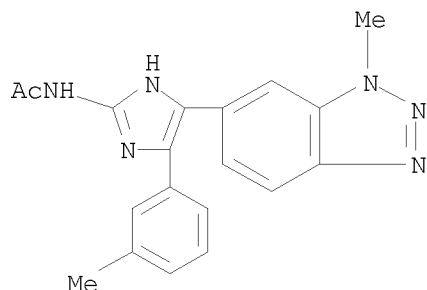
OTHER SOURCE(S): MARPAT 137:279200

AB The title compds. [I; Het = (un)substituted pyrrolyl, imidazolyl, pyrazolyl, oxazolyl, etc.; R2 = H, alkyl, cycloalkyl, etc.; R3 = H, alkyl, Ph, etc.; s = 0-5] which are potent inhibitors of MAP kinases, preferably p38 kinase (no data given), and are useful in the treatment of inflammation, osteoarthritis, rheumatoid arthritis, cancer, reperfusion or ischemia in stroke or heart attack, autoimmune diseases and other disorders, were prepared. Thus, treating a solution of 3-isopropyl-3H-benzotriazole-5-carbaldehyde in THF with concentrate NH4OH followed by addition of piperazine and isocyanide II afforded III.

IT 467234-98-6P  
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of novel benzotriazoles as antiinflammatory agents)

RN 467234-98-6 CAPLUS

CN Acetamide, N-[5-(1-methyl-1H-benzotriazol-6-yl)-4-(3-methylphenyl)-1H-imidazol-2-yl]- (CA INDEX NAME)



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 8 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2002:716272 CAPLUS

DOCUMENT NUMBER: 137:232656

TITLE: Preparation of 5-(phenylheteroaryl)-1,3-dihydro-2-benzimidazolone MAP kinase inhibitors as anti-inflammatory agents

INVENTOR(S): Dombroski, Mark Anthony; Letavic, Michael Anthony; McClure, Kim Francis

PATENT ASSIGNEE(S): Pfizer Products Inc., USA

SOURCE: PCT Int. Appl., 272 pp.

CODEN: PIXXD2

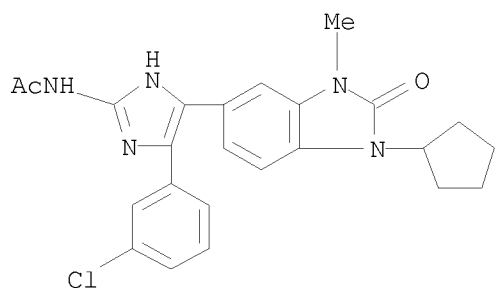
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

## PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002072576	A1	20020919	WO 2002-IB334	20020130 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2440211	A1	20020919	CA 2002-2440211	20020130 <--
AU 2002226639	A1	20020924	AU 2002-226639	20020130 <--
EP 1370557	A1	20031217	EP 2002-716257	20020130 <--
EP 1370557	B1	20051116		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, LO, MK, CY, AL, TR				
BR 2002007957	A	20040225	BR 2002-7957	20020130 <--
JP 2004526727	T	20040902	JP 2002-571492	20020130 <--
AT 309997	T	20051215	AT 2002-716257	20020130
ES 2251582	T3	20060501	ES 2002-716257	20020130
US 20030092749	A1	20030515	US 2002-94717	20020311 <--
US 7056918	B2	20060606		
MX 2003PA08142	A	20031212	MX 2003-PA8142	20030909 <--
PRIORITY APPLN. INFO.:				
			US 2001-274791P	P 20010309
			WO 2002-IB334	W 20020130
OTHER SOURCE(S): CASREACT 137:232656; MARPAT 137:232656				
AB	Title compds. I [wherein Het = (un)substituted pyrrolyl, imidazolyl, pyrazolyl, oxazolyl, isoxazolyl, thiazolyl, or isothiazolyl; R1 and R2 = independently H or (un)substituted (cyclo)alkyl, Ph, heteroaryl, or heterocyclyl; R3 = independently halo, (perhalo)alkyl, (perhalo)cycloalkyl, alkenyl, alkynyl, heterocyclyl(oxy), Ph, OH, (perhalo)alkoxy, OPh, alkylthio, alkyl(amino)sulfonyl, alkylsulfamoyl, carbamoyl, acyl, carboxy, etc.; n = 0-5] were prepared as potent inhibitors of MAP kinases, preferably p38 kinase. For example, (3R)-(-)-1-benzyl-3-aminopyrrolidine was condensed with 1,3-diethyl-2-oxo-2,3-dihydro-1H-benzimidazole-5-carbaldehyde in the presence of MgSO4 in CH2Cl2. Addition of [(4-methylphenylsulfonyl)(m-tolyl)methyl]isocyanide to the 5-(benzylpyrrolidinyliminomethyl)benzimidazolone using DMF and MP-carbonate gave the 5-(m-tolyl)imidazolyl derivative Treatment with Pd/C and HCl in MeOH afforded (R)-II•HCl. All of the compds. of the invention that were tested had an IC50 < 10 µM in TNFα and MAPKAP in vitro assays and an ED50 < mg/kg in an in vivo TNFα assay. I are useful in the treatment of inflammation, osteoarthritis, rheumatoid arthritis, cancer, reperfusion of ischemia in stroke or heart attack, autoimmune diseases, and other disorders (no data).			
IT	459184-45-3P RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (anti-inflammatory agent; preparation of (phenylheteroaryl)benzimidazolone MAP kinase inhibitors as anti-inflammatory agents)			
RN	459184-45-3 CAPLUS			
CN	Acetamide, N-[5-(3-chlorophenyl)-4-(1-cyclopentyl-2,3-dihydro-3-methyl-2-oxo-1H-benzimidazol-5-yl)-1H-imidazol-2-yl]- (CA INDEX NAME)			



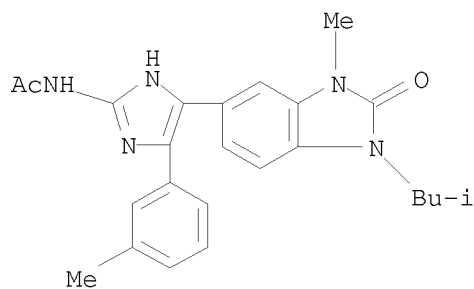
IT 459183-44-9P, N-[5-(1-Isobutyl-3-methyl-2-oxo-2,3-dihydro-1H-benzimidazol-5-yl)-4-(m-tolyl)-1H-imidazol-2-yl]acetamide  
 459183-59-6P 459183-75-6P 459183-83-6P  
 459184-04-4P 459184-13-5P 459184-21-5P  
 459184-53-3P 459184-69-1P 459184-85-1P  
 459184-93-1P 459185-01-4P 459185-09-2P  
 459185-17-2P 459185-25-2P 459185-33-2P  
 459185-41-2P 459185-49-0P 459185-57-0P  
 459185-88-7P 459185-96-7P 459186-03-9P  
 459186-17-5P 459186-24-4P 459186-55-1P  
 459187-09-8P 459187-16-7P 459187-24-7P  
 459187-39-4P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(anti-inflammatory agent; preparation of (phenylheteroaryl)benzimidazolone MAP kinase inhibitors as anti-inflammatory agents)

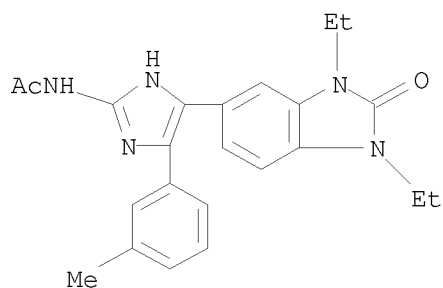
RN 459183-44-9 CAPLUS

CN Acetamide, N-[5-[2,3-dihydro-3-methyl-1-(2-methylpropyl)-2-oxo-1H-benzimidazol-5-yl]-4-(3-methylphenyl)-1H-imidazol-2-yl]- (CA INDEX NAME)

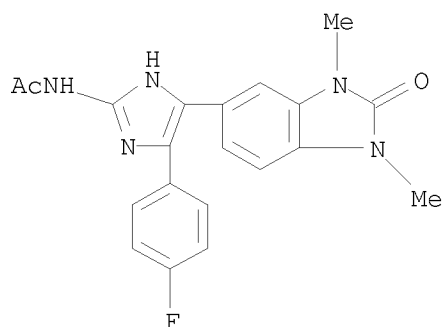


RN 459183-59-6 CAPLUS

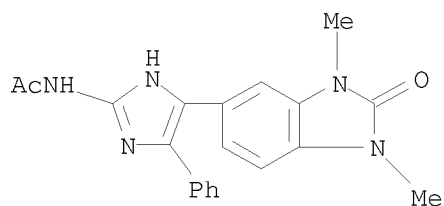
CN Acetamide, N-[5-(1,3-diethyl-2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)-4-(3-methylphenyl)-1H-imidazol-2-yl]- (CA INDEX NAME)



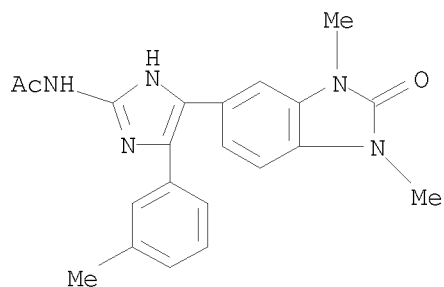
RN 459183-75-6 CAPLUS  
 CN Acetamide, N-[5-(2,3-dihydro-1,3-dimethyl-2-oxo-1H-benzimidazol-5-yl)-4-(4-fluorophenyl)-1H-imidazol-2-yl]- (CA INDEX NAME)



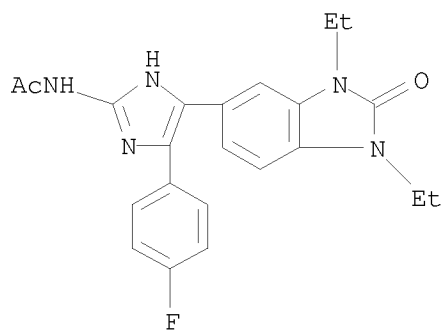
RN 459183-83-6 CAPLUS  
 CN Acetamide, N-[5-(2,3-dihydro-1,3-dimethyl-2-oxo-1H-benzimidazol-5-yl)-4-phenyl-1H-imidazol-2-yl]- (CA INDEX NAME)



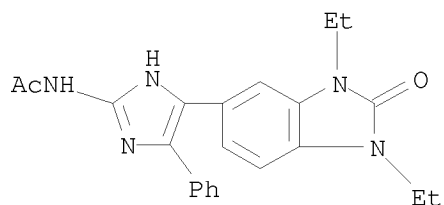
RN 459184-04-4 CAPLUS  
 CN Acetamide, N-[5-(2,3-dihydro-1,3-dimethyl-2-oxo-1H-benzimidazol-5-yl)-4-(3-methylphenyl)-1H-imidazol-2-yl]- (CA INDEX NAME)



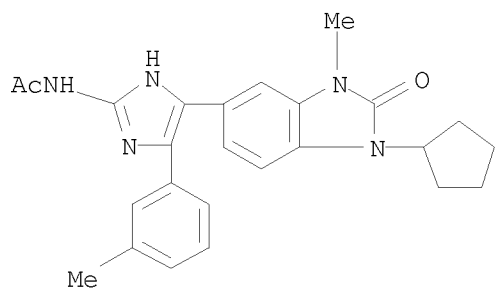
RN 459184-13-5 CAPLUS  
 CN Acetamide, N-[5-(1,3-diethyl-2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)-4-(4-fluorophenyl)-1H-imidazol-2-yl]- (CA INDEX NAME)



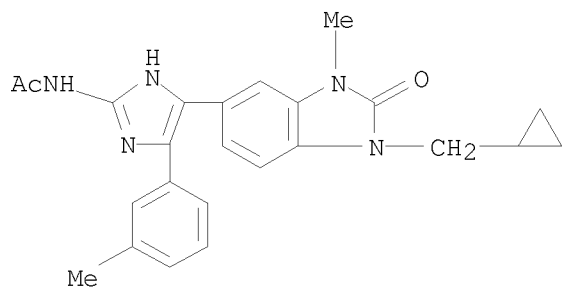
RN 459184-21-5 CAPLUS  
 CN Acetamide, N-[5-(1,3-diethyl-2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)-4-phenyl-1H-imidazol-2-yl]- (CA INDEX NAME)



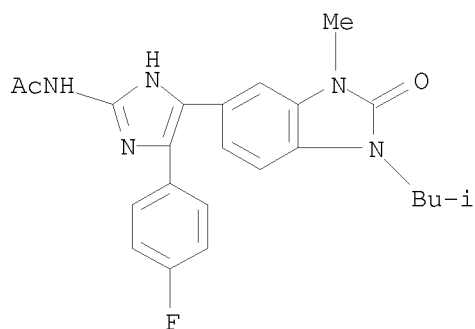
RN 459184-53-3 CAPLUS  
 CN Acetamide, N-[5-(1-cyclopentyl-2,3-dihydro-3-methyl-2-oxo-1H-benzimidazol-5-yl)-4-(3-methylphenyl)-1H-imidazol-2-yl]- (CA INDEX NAME)



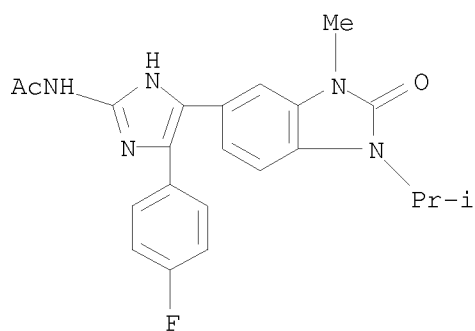
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 CN Acetamide, N-[5-[1-(cyclopropylmethyl)-2,3-dihydro-3-methyl-2-oxo-1H-benzimidazol-5-yl]-4-(3-methylphenyl)-1H-imidazol-2-yl]- (CA INDEX NAME)



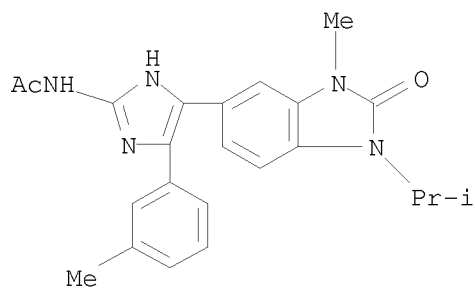
RN 459184-85-1 CAPLUS  
 CN Acetamide, N-[5-[2,3-dihydro-3-methyl-1-(2-methylpropyl)-2-oxo-1H-benzimidazol-5-yl]-4-(4-fluorophenyl)-1H-imidazol-2-yl]- (CA INDEX NAME)



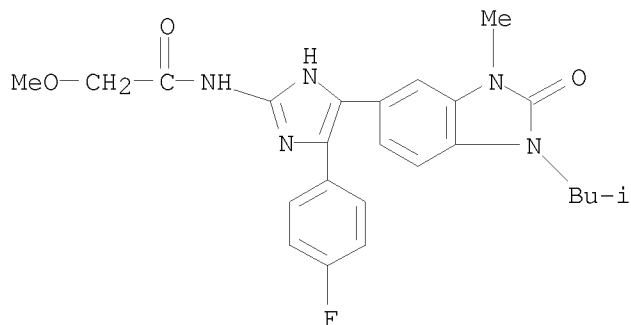
RN 459184-93-1 CAPLUS  
 CN Acetamide, N-[5-[2,3-dihydro-3-methyl-1-(1-methylethyl)-2-oxo-1H-benzimidazol-5-yl]-4-(4-fluorophenyl)-1H-imidazol-2-yl]- (CA INDEX NAME)



RN 459185-01-4 CAPLUS  
 CN Acetamide, N-[5-[2,3-dihydro-3-methyl-1-(1-methylethyl)-2-oxo-1H-benzimidazol-5-yl]-4-(3-methylphenyl)-1H-imidazol-2-yl]- (CA INDEX NAME)

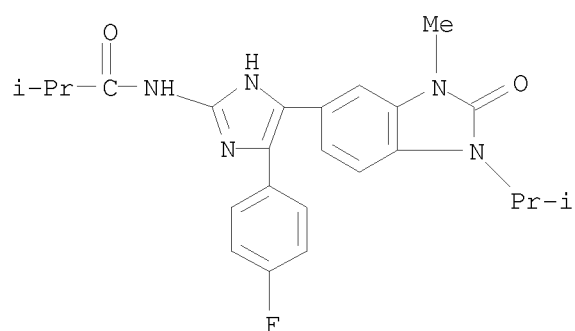


RN 459185-09-2 CAPLUS  
 CN Acetamide, N-[5-[2,3-dihydro-3-methyl-1-(2-methylpropyl)-2-oxo-1H-benzimidazol-5-yl]-4-(4-fluorophenyl)-1H-imidazol-2-yl]-2-methoxy- (CA INDEX NAME)



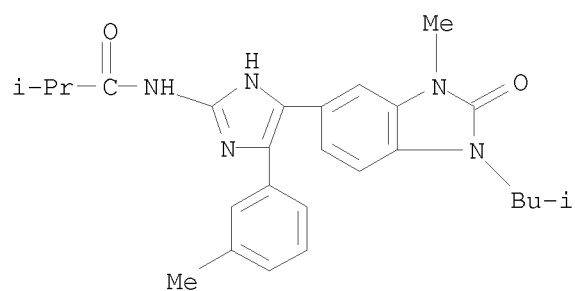
RN 459185-17-2 CAPLUS

CN Propanamide, N-[5-[2,3-dihydro-3-methyl-1-(1-methylethyl)-2-oxo-1H-benzimidazol-5-yl]-4-(4-fluorophenyl)-1H-imidazol-2-yl]-2-methyl- (CA INDEX NAME)



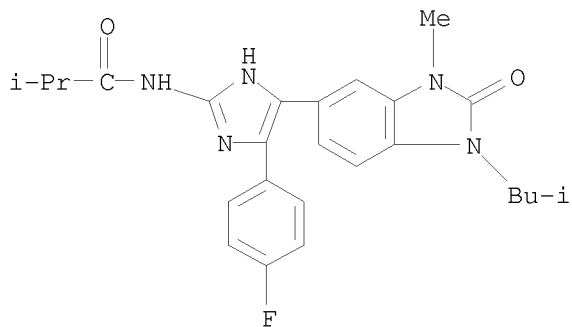
RN 459185-25-2 CAPLUS

CN Propanamide, N-[5-[2,3-dihydro-3-methyl-1-(2-methylpropyl)-2-oxo-1H-benzimidazol-5-yl]-4-(3-methylphenyl)-1H-imidazol-2-yl]-2-methyl- (CA INDEX NAME)



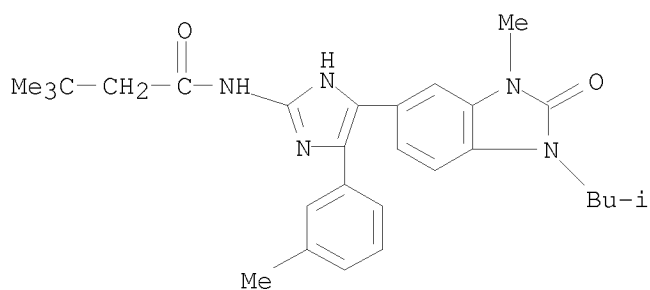
RN 459185-33-2 CAPLUS

CN Propanamide, N-[5-[2,3-dihydro-3-methyl-1-(2-methylpropyl)-2-oxo-1H-benzimidazol-5-yl]-4-(4-fluorophenyl)-1H-imidazol-2-yl]-2-methyl- (CA INDEX NAME)



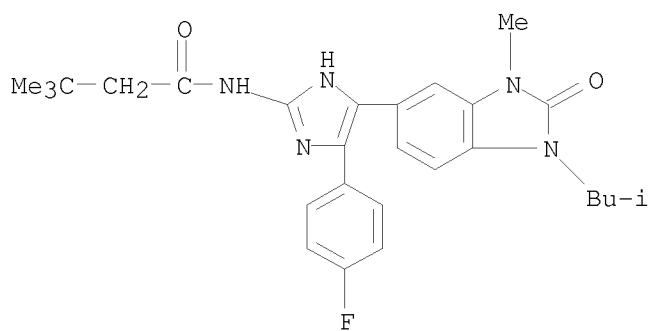
RN 459185-41-2 CAPLUS

CN Butanamide, N-[5-[2,3-dihydro-3-methyl-1-(2-methylpropyl)-2-oxo-1H-benzimidazol-5-yl]-4-(3-methylphenyl)-1H-imidazol-2-yl]-3,3-dimethyl- (CA INDEX NAME)



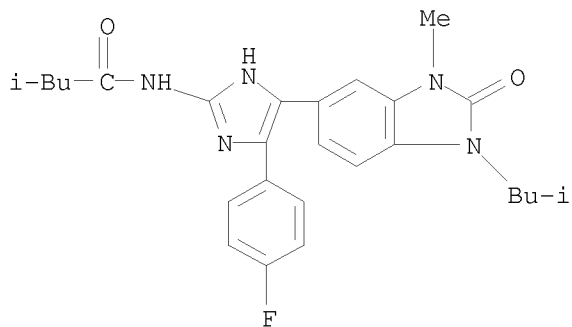
RN 459185-49-0 CAPLUS

CN Butanamide, N-[5-[2,3-dihydro-3-methyl-1-(2-methylpropyl)-2-oxo-1H-benzimidazol-5-yl]-4-(4-fluorophenyl)-1H-imidazol-2-yl]-3,3-dimethyl- (CA INDEX NAME)

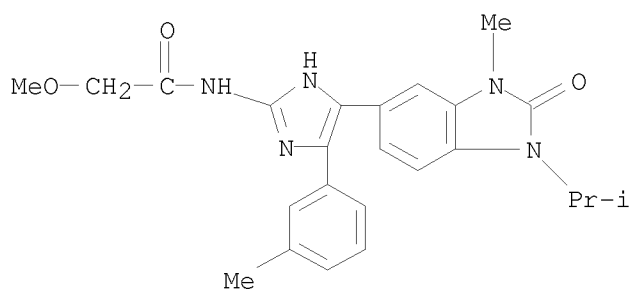


RN 459185-57-0 CAPLUS

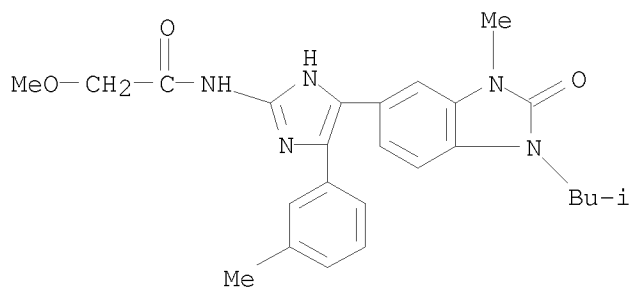
CN Butanamide, N-[5-[2,3-dihydro-3-methyl-1-(2-methylpropyl)-2-oxo-1H-benzimidazol-5-yl]-4-(4-fluorophenyl)-1H-imidazol-2-yl]-3-methyl- (CA INDEX NAME)



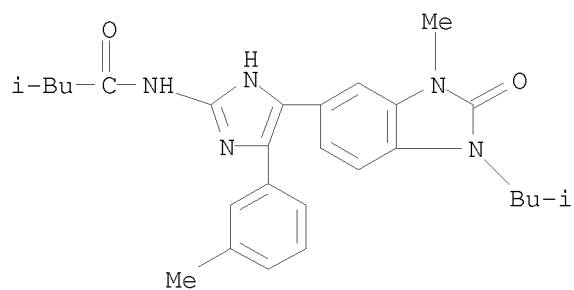
RN 459185-88-7 CAPLUS  
 CN Acetamide, N-[5-[2,3-dihydro-3-methyl-1-(1-methylethyl)-2-oxo-1H-benzimidazol-5-yl]-4-(3-methylphenyl)-1H-imidazol-2-yl]-2-methoxy- (CA INDEX NAME)



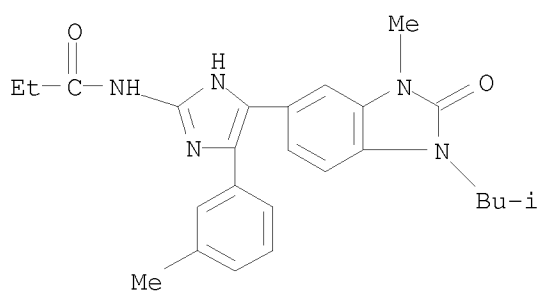
RN 459185-96-7 CAPLUS  
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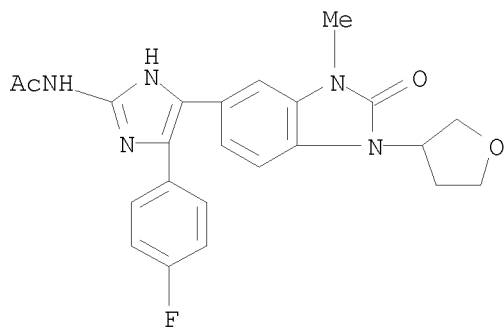
RN 459186-03-9 CAPLUS  
 CN Butanamide, N-[5-[2,3-dihydro-3-methyl-1-(2-methylpropyl)-2-oxo-1H-benzimidazol-5-yl]-4-(3-methylphenyl)-1H-imidazol-2-yl]-3-methyl- (CA INDEX NAME)



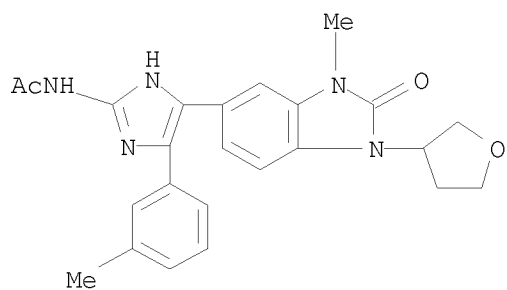
RN 459186-17-5 CAPLUS  
 CN Propanamide, N-[5-[2,3-dihydro-3-methyl-1-(2-methylpropyl)-2-oxo-1H-benzimidazol-5-yl]-4-(3-methylphenyl)-1H-imidazol-2-yl]- (CA INDEX NAME)



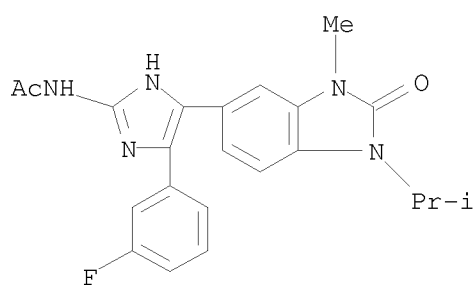
RN 459186-24-4 CAPLUS  
 CN Acetamide, N-[5-[2,3-dihydro-3-methyl-2-oxo-1-(tetrahydro-3-furanyl)-1H-benzimidazol-5-yl]-4-(4-fluorophenyl)-1H-imidazol-2-yl]- (CA INDEX NAME)



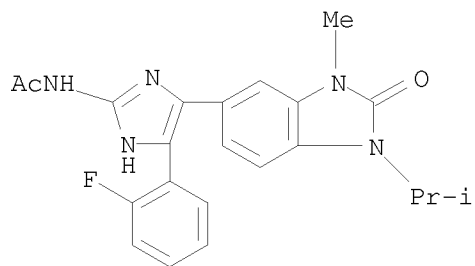
RN 459186-55-1 CAPLUS  
 CN Acetamide, N-[5-[2,3-dihydro-3-methyl-2-oxo-1-(tetrahydro-3-furanyl)-1H-benzimidazol-5-yl]-4-(3-methylphenyl)-1H-imidazol-2-yl]- (CA INDEX NAME)



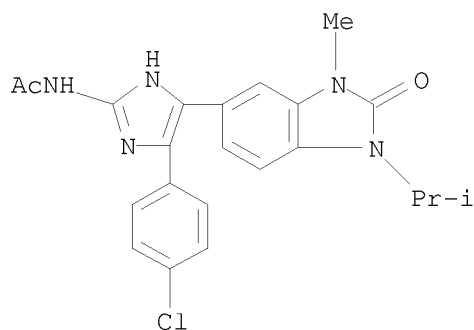
RN 459187-09-8 CAPLUS  
 CN Acetamide, N-[4-[2,3-dihydro-3-methyl-1-(1-methylethyl)-2-oxo-1H-benzimidazol-5-yl]-5-(3-fluorophenyl)-1H-imidazol-2-yl]- (CA INDEX NAME)



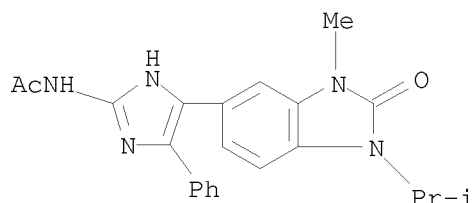
RN 459187-16-7 CAPLUS  
 CN Acetamide, N-[4-[2,3-dihydro-3-methyl-1-(1-methylethyl)-2-oxo-1H-benzimidazol-5-yl]-5-(2-fluorophenyl)-1H-imidazol-2-yl]- (CA INDEX NAME)



RN 459187-24-7 CAPLUS  
 CN Acetamide, N-[4-(4-chlorophenyl)-5-[2,3-dihydro-3-methyl-1-(1-methylethyl)-2-oxo-1H-benzimidazol-5-yl]-1H-imidazol-2-yl]- (CA INDEX NAME)



RN 459187-39-4 CAPLUS  
 CN Acetamide, N-[5-[2,3-dihydro-3-methyl-1-(1-methylethyl)-2-oxo-1H-benzimidazol-5-yl]-4-phenyl-1H-imidazol-2-yl]- (CA INDEX NAME)



REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 9 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2001:283949 CAPLUS  
 DOCUMENT NUMBER: 134:311218  
 TITLE: Synthesis and use of heterocyclic sodium/proton exchange inhibitors  
 INVENTOR(S): Ahmad, Saleem; Wu, Shung C.; O'Neil, Steven V.; Ngu, Khehyong; Atwal, Karnail S.  
 PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA  
 SOURCE: PCT Int. Appl., 221 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001027107	A2	20010419	WO 2000-US27461	20001002 <--
WO 2001027107	A3	20020124		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 6887870	B1	20050503	US 2000-669298	20000925
CA 2388813	A1	20010419	CA 2000-2388813	20001002 <--

EP 1224183	A2	20020724	EP 2000-968723	20001002 <--
EP 1224183	B1	20051228		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
BR 2000014725	A	20030617	BR 2000-14725	20001002 <--
HU 2003000195	A2	20030728	HU 2003-195	20001002 <--
HU 2003000195	A3	20030929		
JP 2003527331	T	20030916	JP 2001-530325	20001002 <--
NZ 517668	A	20040924	NZ 2000-517668	20001002 <--
AT 314364	T	20060115	AT 2000-968723	20001002
ES 2254236	T3	20060616	ES 2000-968723	20001002
IN 2002MN00354	A	20050318	IN 2002-MN354	20020322
ZA 2002002479	A	20040727	ZA 2002-2479	20020327 <--
MX 2002PA03626	A	20030922	MX 2002-PA3626	20020410 <--
NO 2002001717	A	20020610	NO 2002-1717	20020411 <--
US 20050137216	A1	20050623	US 2005-46993	20050131
US 7326705	B2	20080205		

PRIORITY APPLN. INFO.:

US 1999-158755P	P	19991012
US 2000-669298	A3	20000925
WO 2000-US27461	W	20001002

OTHER SOURCE(S): MARPAT 134:311218

AB Compds. of formula I [wherein; n is 1-5; X is N or CR<sup>5</sup>, where R<sup>5</sup> is H, halo, alkenyl, alkynyl, alkoxy, alkyl, aryl or heteroaryl; Z is a heteroaryl group; R<sub>1</sub> is H, alk(en)(yn)yl, alk(enyl)(ynyl)oxy, (aryl or alkyl)3Si, cycloalk(en)yl, (aryl)amino, aryl(alkyl), cycloheteroaryl, etc.; R<sub>2</sub>, R<sub>3</sub> and R<sub>4</sub> are any of the groups set out for R<sub>1</sub> and optionally substituted with 1 to 5 substituents which may be the same or different and when X is N, R<sub>1</sub> is preferably aryl or heteroaryl] are claimed. Several hundred examples are disclosed. Synthesis of II proceeds via cyclopropanation of the cinnamate derived from the olefination between 3,5-dichlorobenzaldehyde and t-butyldiethylphosphonoacetate. The intermediate tert-Bu ester is converted to the corresponding  $\alpha$ -chloroketone and reacted with acetyl guanidine to provide II in a total of 5 steps. Compds. I are said to be sodium/proton exchange inhibitors (NHE). Pharmaceutical combinations are claimed using I and certain antihypertensive agents,  $\beta$ -adrenergic agonists, hypolipidemic agents, antidiabetic agents, antiobesity agents, etc. Compds. I are useful as antianginal and cardioprotective agents and provide a method for preventing or treating angina pectoris, cardiac dysfunction, myocardial necrosis, and arrhythmia.

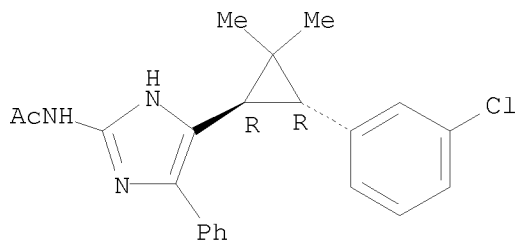
IT 335061-48-8P  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(synthesis and use of heterocyclic sodium/proton exchange inhibitors)

RN 335061-48-8 CAPLUS

CN Acetamide, N-[4-[(1R,3R)-3-(3-chlorophenyl)-2,2-dimethylcyclopropyl]-5-phenyl-1H-imidazol-2-yl]-, rel- (CA INDEX NAME)

Relative stereochemistry.



L15 ANSWER 10 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2000:98527 CAPLUS

DOCUMENT NUMBER: 132:137388

TITLE: Preparation of N-imidazolylalkyl-2-imidazoleamines as histamine H3 receptor ligands

INVENTOR(S): Jegham, Samir; Saady, Mourad; Yaiche, Philippe; Horter, Laurence

PATENT ASSIGNEE(S): Sanofi-Synthelabo, Fr.

SOURCE: PCT Int. Appl., 23 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: French

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000006552	A1	20000210	WO 1999-FR1824	19990726 <--
W:	AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
FR 2781798	A1	20000204	FR 1998-9602	19980728 <--
FR 2781798	B1	20000908		
AU 9949166	A1	20000221	AU 1999-49166	19990726 <--
PRIORITY APPLN. INFO.:			FR 1998-9602	A 19980728
			WO 1999-FR1824	W 19990726

OTHER SOURCE(S): MARPAT 132:137388

AB RZNH(CH<sub>2</sub>)mR1 (R1 = 1H-imidazole-4-yl)[I; R = (un)substituted Ph; Z = (un)substituted 1H-imidazole-5,2-diyl; m = 2-4] were prepared Thus, PhCH(OH)COPh was cyclocondensed with urea and the chlorinated product aminated by H<sub>2</sub>CH<sub>2</sub>Ph to give, after deprotection, 4,5-diphenyl-1H-imidazole-2-amine which was amidated by 1H-imidazole-4-propanoic acid and the product reduced to give I (R = Ph, Z = 3-phenyl-1H-imidazole-5,2-diyl, m = 3). Data for biol. activity of I were given.

IT 256657-13-3P 256657-15-5P 256657-16-6P

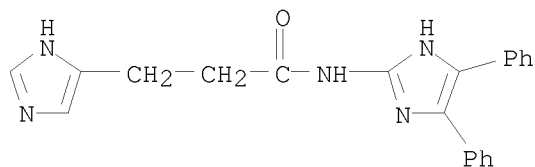
256657-18-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of N-imidazolylalkyl-2-imidazoleamines as histamine H3 receptor ligands)

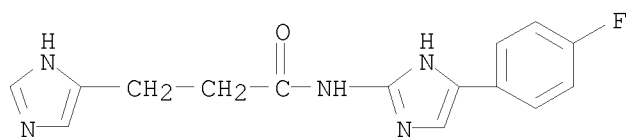
RN 256657-13-3 CAPLUS

CN 1H-Imidazole-5-propanamide, N-(4,5-diphenyl-1H-imidazol-2-yl)-, hydrochloride (1:2) (CA INDEX NAME)

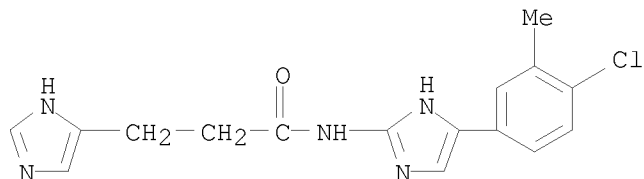


● 2 HCl

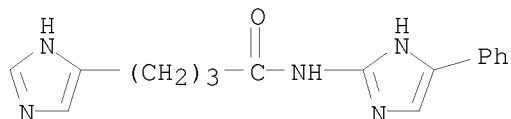
RN 256657-15-5 CAPLUS  
CN 1H-Imidazole-5-propanamide, N-[5-(4-fluorophenyl)-1H-imidazol-2-yl]- (CA INDEX NAME)



RN 256657-16-6 CAPLUS  
CN 1H-Imidazole-5-propanamide, N-[5-(4-chloro-3-methylphenyl)-1H-imidazol-2-yl]- (CA INDEX NAME)



RN 256657-18-8 CAPLUS  
CN 1H-Imidazole-5-butanamide, N-(5-phenyl-1H-imidazol-2-yl)- (CA INDEX NAME)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 11 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1999:723017 CAPLUS

DOCUMENT NUMBER: 131:337034

TITLE: Preparation of  
1-naphthylsulfonyl-4-heteroarylbenzoylpiperazines and  
analogues as Factor Xa inhibitors

INVENTOR(S): Nowak, Thorsten; Preston, John; Rayner, John Wall;  
Smithers, Michael James; Stocker, Andrew

PATENT ASSIGNEE(S): Zeneca Limited, UK

SOURCE: PCT Int. Appl., 39 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9957099	A1	19991111	WO 1999-GB1312	19990427 <--
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 9936207	A	19991123	AU 1999-36207	19990427 <--
EP 1082303	A1	20010314	EP 1999-918179	19990427 <--
EP 1082303	B1	20050126		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
AT 287874	T	20050215	AT 1999-918179	19990427
US 6395731	B1	20020528	US 2000-674563	20001220 <--
PRIORITY APPLN. INFO.:			GB 1998-9349	A 19980502
			WO 1999-GB1312	W 19990427

OTHER SOURCE(S): MARPAT 131:337034

AB Title compds. (I) [where A = 5- or 6-membered monocyclic heteroaryl (un)substituted by 1-3 halo, oxo, CO<sub>2</sub>H, CF<sub>3</sub>, CN, NH<sub>2</sub>, OH, NO<sub>2</sub>, (amino)alkyl, alkoxy(carbonyl), and/or (di)alkylamino; Y = (un)substituted phenylene; Z = (un)substituted piperidine-4,1-diyl or piperazine-1,4-diyl; D and D1 = independently H, alkyl, alkenyl, alkynyl, oxo, or OH; E = F, Cl, or Br] were prepared as antithrombotics and anticoagulants. Thus, 4-(4-imidazolyl)benzoic acid HCl (2-step preparation given) was amidated with 1-(6-chloronaphth-2-ylsulfonyl)piperazine to yield the title imidazolylbenzoylpiperazine (II). The IC<sub>50</sub> values of invention compds. ranged from 0.001 to 0.1 μM for Factor Xa inhibition and were > 40 μM for thrombin inhibition (no individual data given). Data for anticoagulant activity of I in conventional prothrombin time tests were given.

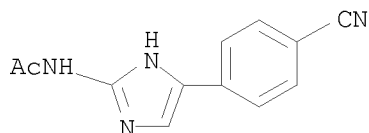
IT 249887-81-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation of 1-naphthylsulfonyl-4-heteroarylbenzoylpiperazines and analogs as Factor Xa inhibitors for treatment of thrombosis mediated diseases and coagulation disorders)

RN 249887-81-8 CAPLUS

CN Acetamide, N-[5-(4-cyanophenyl)-1H-imidazol-2-yl]- (CA INDEX NAME)



REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 12 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1999:659664 CAPLUS

DOCUMENT NUMBER: 131:271809  
 TITLE: Preparation of  
 3-( $\alpha$ -heteroarylaminobenzylidene)-2-indolinones  
 as Cyclin dependent kinase inhibitors  
 INVENTOR(S): Grell, Wolfgang; Walter, Rainer; Heckel, Armin;  
 Himmelsbach, Frank; Wittneben, Helmut; van Meel,  
 Jakobus; Redemann, Norbert; Haigh, Robert  
 PATENT ASSIGNEE(S): Boehringer Ingelheim Pharma K.-G., Germany  
 SOURCE: Ger. Offen., 64 pp.  
 CODEN: GWXXBX  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19815020	A1	19991007	DE 1998-19815020	19980403 <--
US 6043254	A	20000328	US 1999-277063	19990326 <--
WO 9951590	A1	19991014	WO 1999-EP2186	19990330 <--
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG AU 9937034 A 19991025 AU 1999-37034 19990330 <--				
PRIORITY APPLN. INFO.:			DE 1998-19815020	A 19980403
			US 1998-86733P	P 19980526
			WO 1999-EP2186	W 19990330

OTHER SOURCE(S): MARPAT 131:271809

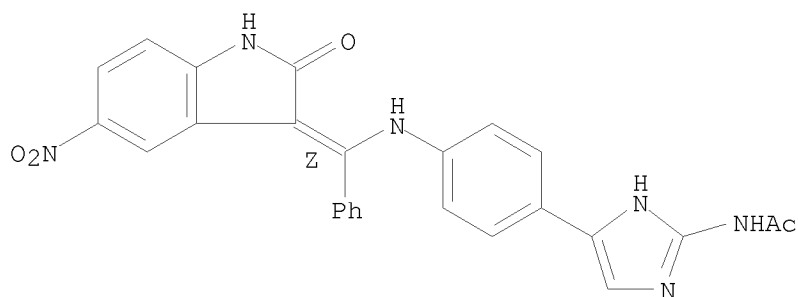
AB Title compds. [I; R = H; R1 = H, halo, NO<sub>2</sub>, (alkanoyl)amino, etc.; R2 = (un)substituted Ph; R4 = NHR<sub>3</sub>; R3 = heteroannelated Ph, heteroaryllalk(en)ylphenyl, etc.] were prepared Thus, 2-indolinone was N-acetylated and the product condensed with PhC(OEt)<sub>3</sub> to give I (R1 = H, R2 = Ph) (II; R = Ac, R4 = OEt) which was condensed with 5-aminoindole to give II (R = H, R4 = 5-indolylamino). Data for biol. activity of I were given.

IT 245546-35-4P 245546-36-5P  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of 3-( $\alpha$ -heteroarylaminobenzylidene)-2-indolinones as cyclin dependent kinase inhibitors)

RN 245546-35-4 CAPLUS

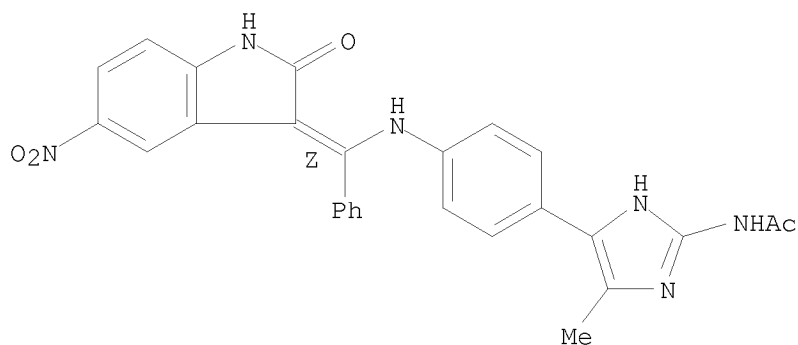
CN Acetamide, N-[5-[4-[[ (Z)-(1,2-dihydro-5-nitro-2-oxo-3H-indol-3-ylidene)phenylmethyl]amino]phenyl]-1H-imidazol-2-yl]- (CA INDEX NAME)

Double bond geometry as shown.

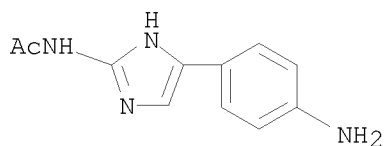


RN 245546-36-5 CAPLUS  
 CN Acetamide, N-[5-[4-[(Z)-(1,2-dihydro-5-nitro-2-oxo-3H-indol-3-ylidene)phenylmethyl]amino]phenyl]-4-methyl-1H-imidazol-2-yl]- (CA INDEX NAME)

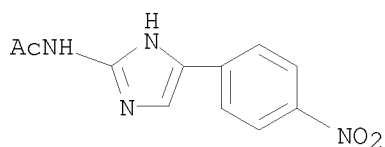
Double bond geometry as shown.



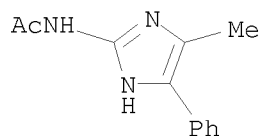
IT 96139-64-9P 96139-70-7P 160072-51-5P  
 245546-86-5P 245546-87-6P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation of 3-( $\alpha$ -heteroarylaminobenzylidene)-2-indolinones as cyclin dependent kinase inhibitors)  
 RN 96139-64-9 CAPLUS  
 CN Acetamide, N-[5-(4-aminophenyl)-1H-imidazol-2-yl]- (CA INDEX NAME)



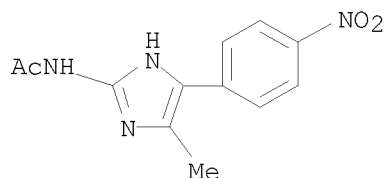
RN 96139-70-7 CAPLUS  
 CN Acetamide, N-[5-(4-nitrophenyl)-1H-imidazol-2-yl]- (CA INDEX NAME)



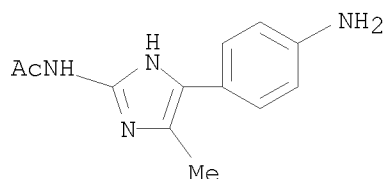
RN 160072-51-5 CAPLUS  
CN Acetamide, N-(4-methyl-5-phenyl-1H-imidazol-2-yl)- (CA INDEX NAME)



RN 245546-86-5 CAPLUS  
CN Acetamide, N-[4-methyl-5-(4-nitrophenyl)-1H-imidazol-2-yl]- (CA INDEX NAME)



RN 245546-87-6 CAPLUS  
CN Acetamide, N-[5-(4-aminophenyl)-4-methyl-1H-imidazol-2-yl]- (CA INDEX NAME)



L15 ANSWER 13 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1999:109589 CAPLUS

DOCUMENT NUMBER: 130:237506

TITLE: Synthesis of novel 4,5-diphenylthiazole derivatives as potential acyl-CoA : cholesterol O-acyltransferase inhibitors

AUTHOR(S): Romeo, G.; Salerno, L.; Milla, P.; Siracusa, M.; Cattel, L.; Russo, Filippo

CORPORATE SOURCE: Dip. Scienze Farmaceutiche, Univ. Catania, Catania, I-95125, Italy

SOURCE: Pharmazie (1999), 54(1), 19-23

CODEN: PHARAT; ISSN: 0031-7144

PUBLISHER: Govi-Verlag Pharmazeutischer Verlag

DOCUMENT TYPE: Journal

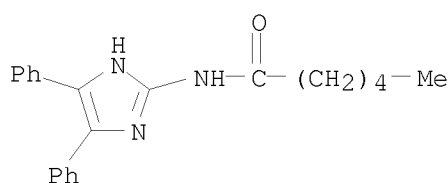
LANGUAGE: English

OTHER SOURCE(S): CASREACT 130:237506

AB Several N-(4,5-diphenylthiazol-2-yl)-N'-aryl- or -alkyl-(thio)ureas and N-(4,5-diphenylthiazol-2-yl)alkanamides were prepared as potential acyl-CoA : cholesterol O-acyltransferase (ACAT) inhibitors. Synthesis was accomplished by reaction of 2-amino-4,5-diphenylthiazole with suitable isocyanates, isothiocyanates, or acyl chlorides. Some analogs without a 5-Ph substituent or both the Ph groups in 4- and 5-position of the thiazole ring were also prepared. Moreover, some bio-isosteres of the title

compds. in which the thiazole ring was replaced by an imidazole were synthesized starting from 2-amino-4,5-diphenyl-1H-imidazole. The ability of synthesized compds. to inhibit ACAT was evaluated in vitro by measuring the formation of cholesteryl[14C]oleate from cholesterol and [1-14C]oleoyl-CoA in rat liver microsomes. Among the tested compds., only some thiazole ureas were able to inhibit ACAT in a reasonable degree. N-(4,5-diphenylthiazol-2-yl)-N'-[2,6-bis(2-methylethyl)phenyl]urea and N-(4,5-diphenylthiazol-2-yl)-N'-butylurea were the most active compds. in the series showing IC50 values in the low micromolar range.

IT 221389-49-7P  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)  
 (preparation of phenylthiazoles cholesterol O-acyltransferase inhibitors)  
 RN 221389-49-7 CAPLUS  
 CN Hexanamide, N-(4,5-diphenyl-1H-imidazol-2-yl)- (CA INDEX NAME)



REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 14 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1998:217660 CAPLUS  
 DOCUMENT NUMBER: 128:277027  
 ORIGINAL REFERENCE NO.: 128:54715a,54718a  
 TITLE: Silver halide photographic material and its processing method providing superior silver tone  
 INVENTOR(S): Yamashita, Hiroshi  
 PATENT ASSIGNEE(S): Konica Co., Japan  
 SOURCE: Jpn. Kokai Tokkyo Koho, 33 pp.  
 CODEN: JKXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 10090821	A	19980410	JP 1996-244931	19960917 <--
PRIORITY APPLN. INFO.:			JP 1996-244931	19960917
OTHER SOURCE(S): MARPAT 128:277027				

AB The material comprises  $\geq 1$  Ag halide emulsion layer on  $\geq 1$  side of a support and  $\geq 1$  hydrophilic colloid layer containing a leuco dye producing blue color in reaction with an oxidized developer and a branched cyclodextrin and/or a cyclodextrin polymer. The material is processed with a developer containing ascorbic acid-type compound Q1C(:Q3)CR1:CR2Q2 (I; R1, R2 = OH, amino, acylamino, alkylsulfonylamino, arylsulfonylamino, alkoxycarbonylamino, mercapto, alkylthio; Q1, Q2 = OH, CO2H, alkoxy, hydroxyalkyl, carboxyalkyl, sulfo, sulfoalkyl, amino, aminoalkyl, alkyl, aryl, non-metallic atoms required to form a 5- to 8-membered ring with a carbon substituted with R1, R2, and Q3; Q3 = O, NR3; R3 = H, OH, alkyl, acyl, hydroxyalkyl, sulfoalkyl, carboxyalkyl) and an auxiliary developer. Alternatively, the material without the

cyclodextrin-based component is processed with a developer containing I, an auxiliary developer, a branched cyclodextrin and/or a cyclodextrin polymer. The material processed by the method shows superior silver tone and stable photog. properties even in running processing with lower replenishment of an ascorbic acid and its derivative instead of a hydroquinone.

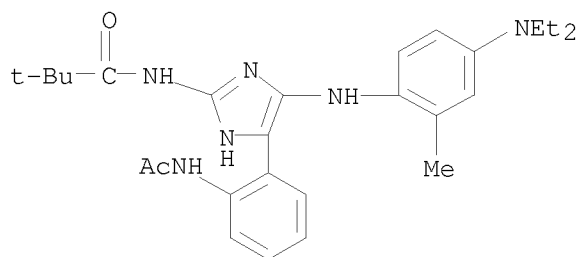
IT 205577-10-2

RL: MOA (Modifier or additive use); USES (Uses)

(leuco dye; silver halide emulsion containing blue-color-forming leuco dye reactive to oxidized photog. developer)

RN 205577-10-2 CAPLUS

CN Propanamide, N-[4-[2-(acetyl amino)phenyl]-5-[[4-(diethylamino)-2-methylphenyl]amino]-1H-imidazol-2-yl]-2,2-dimethyl- (CA INDEX NAME)



L15 ANSWER 15 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1996:472632 CAPLUS

DOCUMENT NUMBER: 125:127626

ORIGINAL REFERENCE NO.: 125:23665a, 23668a

TITLE: Silver halide photographic material containing anilinoimidazole to develop dye image with high spectral absorption

INVENTOR(S): Ookawa, Atsuhiko; Sakai, Minoru

PATENT ASSIGNEE(S): Fuji Photo Film Co Ltd, Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 22 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 08122960	A	19960517	JP 1994-263792	19941027 <--
JP 3505240	B2	20040308		

PRIORITY APPLN. INFO.: JP 1994-263792 19941027

AB The claimed photog. material having, on a support,  $\geq 1$  light-sensitive Ag halide emulsion layer(s) contains an imidazole compound substituted by an anilino group (H atom on NH group is unsubstituted) at 2- or 4-site. Preferable imidazole derivative is represented by the formula I (R1-4 = H, nonmetal substituent; X = OH, NR5R6; R5, R6 = H, alkyl, aryl, heterocyclic group; A, B = nonmetal substituent). The compound is a leuco dye with high dye developability and the developed dye has a high spectral absorbance.

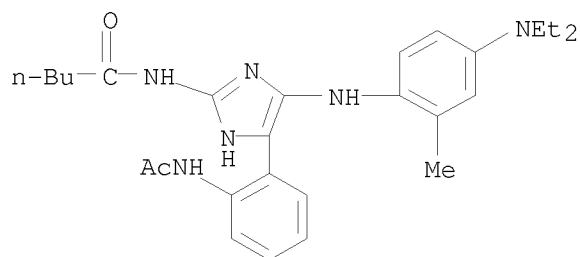
IT 179421-93-3P

RL: DEV (Device component use); PNU (Preparation, unclassified); PREP

(Preparation); USES (Uses)

(silver halide photog. material containing anilinoimidazole to develop dye image with high spectral absorption)

RN 179421-93-3 CAPLUS  
 CN Pentanamide, N-[4-[2-(acetylamino)phenyl]-5-[[4-(diethylamino)-2-methylphenyl]amino]-1H-imidazol-2-yl]- (CA INDEX NAME)



L15 ANSWER 16 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1995:183280 CAPLUS  
 DOCUMENT NUMBER: 122:55805  
 ORIGINAL REFERENCE NO.: 122:10814h,10815a  
 TITLE: A Simple and Practical Synthesis of 2-Aminoimidazoles  
 AUTHOR(S): Little, Thomas L.; Webber, Stephen E.  
 CORPORATE SOURCE: Agouron Pharmaceuticals Inc., San Diego, CA, 92121, USA

SOURCE: Journal of Organic Chemistry (1994), 59(24), 7299-305

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 122:55805

AB A new and simple two-step procedure to synthesize 2-aminoimidazoles (2-AI's) from readily available materials has been developed. The cyclization reaction of  $\alpha$ -halo ketones  $\text{RCOCHR}_1\text{X}$  [ $\text{R} = \text{Me, Et, CMe}_3, \text{Ph, 4-BrC}_6\text{H}_4$ , etc.,  $\text{R}_1 = \text{H, Me, Ph, RR}_1 = (\text{CH}_2)_3, (\text{CH}_2)_4, \text{X} = \text{Cl, Br}$ ] and N-acetylguanidine in acetonitrile (MeCN) at reflux, or in DMF at ambient temperature, gives 4(5)-substituted and 4,5-disubstituted N-(1H-imidazol-2-yl)acetamides I, which are then hydrolyzed to their resp. 2-AI's. In general, the purified products were isolated in good yields. We have prepared several examples and have demonstrated the usefulness of this method by its application in the total synthesis of 2-aminohistamine, an interesting histamine analog, and oroidin (II), a marine natural product isolated from various sponges.

IT 160041-64-5P 160041-65-6P 160041-66-7P

160041-67-8P 160041-68-9P 160041-69-0P

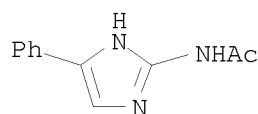
160072-51-5P 160072-52-6P 160072-53-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of aminoimidazoles, aminohistamine, and oroidin by cyclization of carbonyl with acetylguanidine)

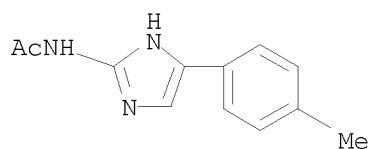
RN 160041-64-5 CAPLUS

CN Acetamide, N-(5-phenyl-1H-imidazol-2-yl)- (CA INDEX NAME)



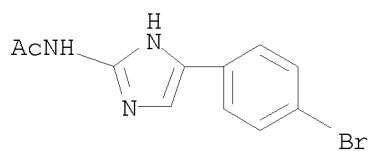
RN 160041-65-6 CAPLUS

CN Acetamide, N-[5-(4-methylphenyl)-1H-imidazol-2-yl]- (CA INDEX NAME)



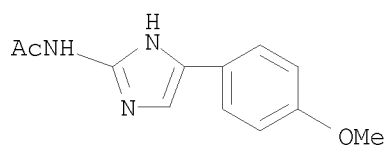
RN 160041-66-7 CAPLUS

CN Acetamide, N-[5-(4-bromophenyl)-1H-imidazol-2-yl]- (CA INDEX NAME)



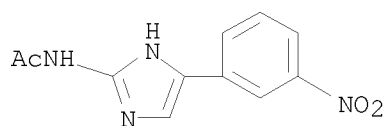
RN 160041-67-8 CAPLUS

CN Acetamide, N-[5-(4-methoxyphenyl)-1H-imidazol-2-yl]- (CA INDEX NAME)



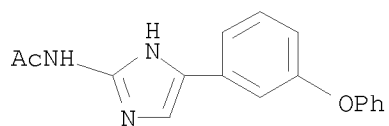
RN 160041-68-9 CAPLUS

CN Acetamide, N-[5-(3-nitrophenyl)-1H-imidazol-2-yl]- (CA INDEX NAME)



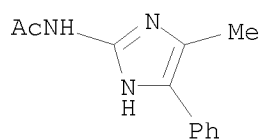
RN 160041-69-0 CAPLUS

CN Acetamide, N-[5-(3-phenoxyphenyl)-1H-imidazol-2-yl]- (CA INDEX NAME)

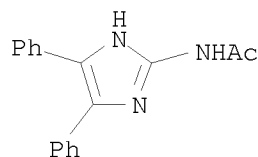


RN 160072-51-5 CAPLUS

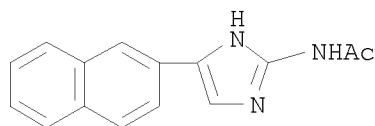
CN Acetamide, N-(4-methyl-5-phenyl-1H-imidazol-2-yl)- (CA INDEX NAME)



RN 160072-52-6 CAPLUS  
CN Acetamide, N-(4,5-diphenyl-1H-imidazol-2-yl)- (CA INDEX NAME)



RN 160072-53-7 CAPLUS  
CN Acetamide, N-[5-(2-naphthalenyl)-1H-imidazol-2-yl]- (CA INDEX NAME)



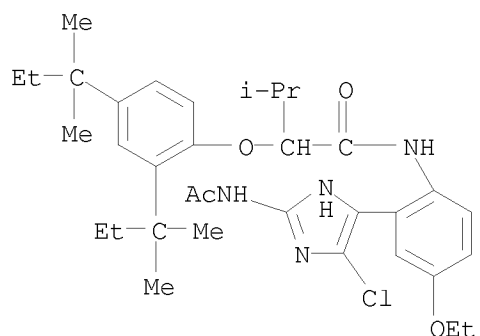
L15 ANSWER 17 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 1992:540469 CAPLUS  
DOCUMENT NUMBER: 117:140469  
ORIGINAL REFERENCE NO.: 117:24183a,24186a  
TITLE: Cyan coupler-containing photographic material  
INVENTOR(S): Nakayama, Noritaka; Uchida, Taku; Masukawa, Toyooki  
PATENT ASSIGNEE(S): Konica Co., Japan  
SOURCE: Jpn. Kokai Tokkyo Koho, 13 pp.  
CODEN: JKXXAF  
DOCUMENT TYPE: Patent  
LANGUAGE: Japanese  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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JP 03284746	A	19911216	JP 1990-86760	19900330 <--
PRIORITY APPLN. INFO.:			JP 1990-86760	19900330

AB In the title photog. material containing  $\geq 1$  Ag halide emulsion layers,  $\geq 1$  of the Ag halide emulsion layer contains a cyan coupler (I) [R = H, substituent; L = divalent linking group; R1 = proton donor which may H-bond with N of the parent ring; R2 = substituent; m = 1-4; X = H, group releasable on coupling with an oxidized color developing agent]. The cyan dye produced by this coupler has good spectral absorption characteristics with sharp cutoff at the shortwave side, unsym. absorption is not observed in the blue and green regions, and color reproducibility is superior.

IT 143316-84-1P  
RL: PREP (Preparation)  
(preparation of, as photog. cyan coupler)

RN 143316-84-1 CAPLUS  
CN Butanamide, N-[2-[2-(acetylamino)-5-chloro-1H-imidazol-4-yl]-4-ethoxyphenyl]-2-[2,4-bis(1,1-dimethylpropyl)phenoxy]-3-methyl- (CA INDEX NAME)



L15 ANSWER 18 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1992:13220 CAPLUS

DOCUMENT NUMBER: 116:13220

ORIGINAL REFERENCE NO.: 116:2279a,2282a

TITLE: Heat developable color photographic material

INVENTOR(S): Miura, Akio; Masukawa, Toyooki; Komamura, Tawara

PATENT ASSIGNEE(S): Konica Co., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 31 pp.

CODEN: JKXXAF

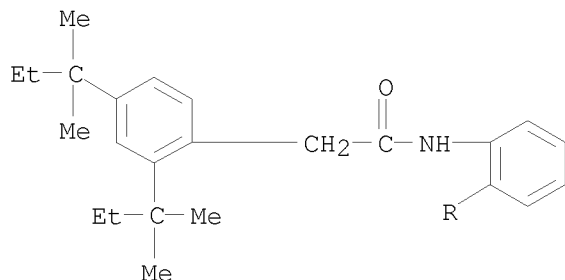
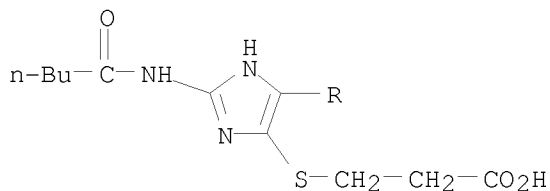
DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 03089343	A	19910415	JP 1989-227154	19890901 <--
PRIORITY APPLN. INFO.:			JP 1989-227154	19890901
AB The title material on a support comprises photosensitive silver halide, a reducing agent, a binder, and cyan dye-forming coupler I (A, B = organic group connected to the imidazole ring by the C, N, O, or S atom; X = H, group which is released upon coupling reaction with the oxidized form of the reducing agent). I (A = Q1, B = Q2; X = Q3) is an example of the general structure I defined above. The use of I provides stable cyan dyes and gives excellent cyan dye images.				
IT 137590-60-4				
RL: USES (Uses)				
(cyan dye-forming coupler, in photog. material)				
RN 137590-60-4 CAPLUS				
CN Propanoic acid, 3-[[4-[2-[[2-[2,4-bis(1,1-dimethylpropyl)phenyl]acetyl]amino]phenyl]-2-[(1-oxopentyl)amino]-1H-imidazol-5-yl]thio]- (CA INDEX NAME)				



L15 ANSWER 19 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN

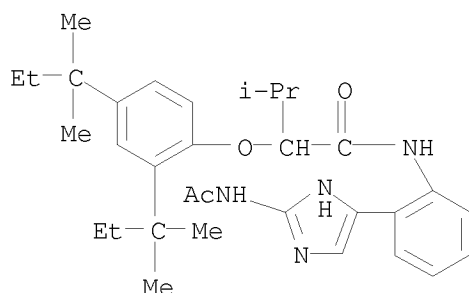
ACCESSION NUMBER: 1990:408016 CAPLUS  
 DOCUMENT NUMBER: 113:8016  
 ORIGINAL REFERENCE NO.: 113:1505a,1508a  
 TITLE: Imidazole dyes for thermal-transfer printing inks  
 INVENTOR(S): Uchida, Taku; Masukawa, Toyooki; Nakayama, Noritaka  
 PATENT ASSIGNEE(S): Konica Co., Japan  
 SOURCE: Jpn. Kokai Tokkyo Koho, 11 pp.  
 CODEN: JKXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 02028264	A	19900130	JP 1988-177357	19880715 <--
PRIORITY APPLN. INFO.:			JP 1988-177357	19880715
OTHER SOURCE(S): MARPAT 113:8016				

AB The title dyes, with lower undesired absorption than indoaniline dyes and better heat and light resistance than cyanine dyes, have the general formula I [R1, R2 = H, (un)substituted alkyl; R1,R2 = 5- or 6-membered ring member; R3-6 = H, halogen, (un)substituted alkyl, alkoxy; R7 = H, (un)substituted alkyl, aryl, R11CO, R11O2C, R12NHCO, R13R14NCO, R11SO2, R11OSO2, R12NHCO, R13R14NSO2; R11 = H, (un)substituted alkyl; R12 = (un)substituted aryl, heterocyclic, R13, R14 = (un)substituted alkyl; X = CO, SO2, NHCO; R8 = (un)substituted alkyl, Q; R9, R10 = monovalent group; n = 0-4; n = 0-5]. Benzaldehyde guanyl hydrazone and 2-[2-(2,4-di-tert-amylphenoxy)isopentanamido]phenacylbromide in CHCl3 were refluxed for 10 min and stirred at room temperature for 1 h to give 2-benzylidenehydrazino-4-[2-[2-(2,4-di-tert-amylphenoxy)isopentanaido]phenyl]imidazole, which was stirred with Zn/HCl in acetone to give 2-amino-4-[2-[2-(2,4-di-tert-amylphenoxy)isopentanamido]phenyl]imidazole. This product was treated with BzCl in the presence of NaOAc in EtOAc to give 2-amino-3-benzoyl-4-[2-[2-(2,4-di-tert-amylphenoxy)isopentanamido]phenyl]imidazole, which was then heated with p-MeC6H4SO3H in PhNO2 at 150° for 1 h to give 2-benzoylamino-4-[2-[2-(2,4-di-tert-

amylphenoxy)isopentanamido]phenyl]imidazole, which was then dissolved in EtOAc, stirred with aqueous K<sub>2</sub>CO<sub>3</sub>, treated with aqueous 4-amino-3-methyl-N-methyl-N-( $\beta$ -methanesulfonamidomethyl)aniline sulfate, then with 10% aqueous K<sub>2</sub>S<sub>2</sub>O<sub>8</sub> to give I [R<sub>1</sub> = Et; R<sub>2</sub> = CH<sub>2</sub>CH<sub>2</sub>NHSO<sub>2</sub>Me; R<sub>2</sub> = Me; R<sub>4</sub> = R<sub>5</sub> = R<sub>6</sub> = R<sub>9</sub> = H; R<sub>7</sub> = 2-(2,4-di-tert-amylphenoxyisopropanoyl)].

IT 127698-35-5P  
 RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)  
 (manufacture and reaction of, with aniline derivs.)  
 RN 127698-35-5 CAPLUS  
 CN Butanamide, N-[2-[2-(acetlamino)-1H-imidazol-5-yl]phenyl]-2-[2,4-bis(1,1-dimethylpropyl)phenoxy]-3-methyl- (CA INDEX NAME)



L15 ANSWER 20 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1987:32967 CAPLUS

DOCUMENT NUMBER: 106:32967

ORIGINAL REFERENCE NO.: 106:5527a,5530a

TITLE: Heterocyclic rearrangements. Rearrangement of N-(1,2,4-oxadiazol-3-yl)- $\beta$ -enamino ketones to pyrimidine N-oxides

AUTHOR(S): Vivona, Nicolo; Buscemi, Silvestre; Frenna, Vincenzo; Ruccia, Michele

CORPORATE SOURCE: Inst. Org. Chem., Univ. Palermo, Palermo, 90123, Italy

SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1986), (1), 17-19

CODEN: JCPRB4; ISSN: 0300-922X

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 106:32967

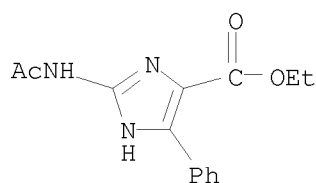
AB The behavior of oxadiazolylenamino ketones I (R, R<sub>1</sub> = Me, Ph; R<sub>2</sub> = Me, Ph, OEt) towards rearrangement has been investigated. In the presence of anionic reagents in ethanol solution, they rearrange to pyrimidine N-oxides II (R<sub>3</sub> = Me, Ph). The synthesis and hydrolytic ring opening of an oxadiazolopyrimidinium system III is also reported.

IT 55729-99-2P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)

RN 55729-99-2 CAPLUS

CN 1H-Imidazole-4-carboxylic acid, 2-(acetlamino)-5-phenyl-, ethyl ester (9CI) (CA INDEX NAME)



L15 ANSWER 21 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1985:185082 CAPLUS

DOCUMENT NUMBER: 102:185082

ORIGINAL REFERENCE NO.: 102:29037a,29040a

TITLE: Amidine derivatives of 2-substituted 4-phenylimidazole

INVENTOR(S): Bietti, Giuseppe; Cereda, Enzo; Donetti, Arturo;

Giachetti, Antonio; Pagani, Ferdinando

PATENT ASSIGNEE(S): Istituto De Angeli S.p.A., Italy

SOURCE: Eur. Pat. Appl., 43 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 131973	A1	19850123	EP 1984-200659	19840508 <--
EP 131973	B1	19890802		
R: AT, BE, CH, DE, FR, IT, LI, LU, NL, SE				
AT 45149	T	19890815	AT 1984-200659	19840508 <--
US 4649150	A	19870310	US 1984-610958	19840516 <--
FI 8402432	A	19850119	FI 1984-2432	19840615 <--
JP 60038367	A	19850227	JP 1984-142099	19840709 <--
DD 232696	A5	19860205	DD 1984-265319	19840716 <--
PL 143303	B1	19880229	PL 1984-248779	19840716 <--
IL 72417	A	19880331	IL 1984-72417	19840716 <--
PL 143732	B1	19880331	PL 1984-254625	19840716 <--
DK 8403500	A	19850119	DK 1984-3500	19840717 <--
NO 8402921	A	19850121	NO 1984-2921	19840717 <--
NO 162857	B	19891120		
NO 162857	C	19900228		
HU 34959	A2	19850528	HU 1984-2781	19840717 <--
HU 193292	B	19870928		
GB 2149395	A	19850612	GB 1984-18149	19840717 <--
GB 2149395	B	19861126		
ZA 8405490	A	19860326	ZA 1984-5490	19840717 <--
SU 1322979	A3	19870707	SU 1984-3770847	19840717 <--
CA 1257274	A1	19890711	CA 1984-459030	19840717 <--
AU 8430800	A	19850124	AU 1984-30800	19840718 <--
AU 565292	B2	19870910		
CS 244141	B2	19860717	CS 1984-5542	19840718 <--
SU 1313345	A3	19870523	SU 1985-3844125	19850129 <--
CS 244150	B2	19860717	CS 1985-2801	19850416 <--
PRIORITY APPLN. INFO.:			IT 1983-22110	A 19830718
			EP 1984-200659	A 19840508
			CS 1984-5542	A3 19840718

OTHER SOURCE(S): MARPAT 102:185082

AB Forty-four (amidinophenyl)imidazoles I [R = alkyl, OH, alkoxy, SH, alkylthio, halo, alkylsulfinyl, alkylsulfonyl, SO<sub>2</sub>NH<sub>2</sub>, (di)(alkyl)amino, acylamino, Ph; R<sub>1</sub>, R<sub>2</sub> = H, alkyl; R<sub>3</sub> = alkyl optionally containing 1 hetero atom such as O, S, or N, alkenyl, alkynyl, cyano, cycloalkyl, cycloaliph.

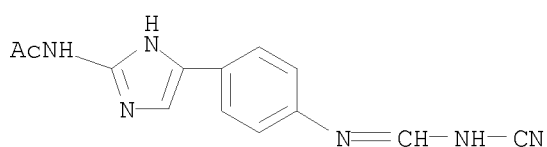
alkyl, (un)substituted aryl, aralkyl, heterocyclylalkyl, heterocyclyl; R4 = H, alkyl, alkoxy, halo, cyano, CONH2] were prepared Thus, 4-O2NC6H4COCH2Br in water was treated with AcNH2 at 140° for 8 h to give phenylimidazole II (R5 = NO2), which was catalytically reduced to II (R5 = NH2). The latter compound was condensed with EtOCH:NCN to give II (R5 = N:CHNHCN), which was treated with EtNH2 to give II (R5 = N:CHNHET)(III). III inhibited histamine-induced tachycardia in isolated guinea pig atria with an EC50 of  $1.5 \times 10^{-7}M$ .

IT 96139-96-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and reaction of, with isopropylamine)

RN 96139-96-7 CAPLUS

CN Acetamide, N-[5-[4-[[[(cyanoamino)methylene]amino]phenyl]-1H-imidazol-2-yl]- (CA INDEX NAME)

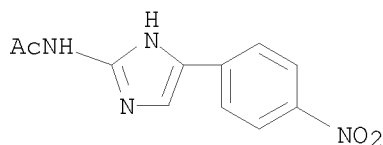


IT 96139-70-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and reduction of)

RN 96139-70-7 CAPLUS

CN Acetamide, N-[5-(4-nitrophenyl)-1H-imidazol-2-yl]- (CA INDEX NAME)



IT 96154-06-2P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

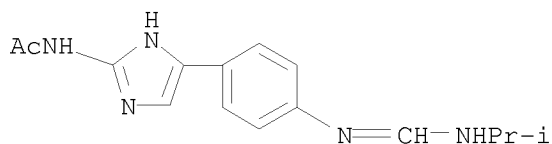
RN 96154-06-2 CAPLUS

CN Acetamide, N-[4-[4-[[[(1-methylethyl)amino]methylene]amino]phenyl]-1H-imidazol-2-yl]-, (2Z)-2-butenedioate (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 96154-05-1

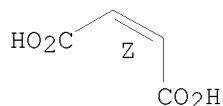
CMF C15 H19 N5 O



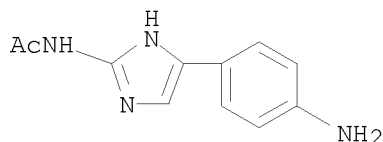
CM 2

CRN 110-16-7  
CMF C4 H4 O4

Double bond geometry as shown.



IT 96139-64-9P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation, hydride reduction, and reaction of, with cyanoformimidate)  
RN 96139-64-9 CAPLUS  
CN Acetamide, N-[5-(4-aminophenyl)-1H-imidazol-2-yl]- (CA INDEX NAME)



L15 ANSWER 22 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1975:112006 CAPLUS

DOCUMENT NUMBER: 82:112006

ORIGINAL REFERENCE NO.: 82:17899a,17902a

TITLE: Mononuclear heterocyclic rearrangements. VI.  
Conversion of 1,2,4-oxadiazoles into imidazoles

AUTHOR(S): Ruccia, M.; Vivona, N.; Cusmano, G.

CORPORATE SOURCE: Fac. Sci., Univ. Palermo, Palermo, Italy

SOURCE: Tetrahedron (1974), 30(21), 3859-64

CODEN: TETRAB; ISSN: 0040-4020

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 82:112006

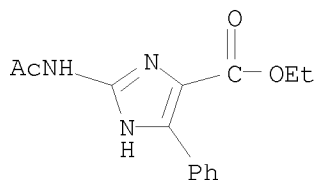
AB Condensation of aminooxadiazoles with  $\beta$ -oxo ketones or esters gave  $\beta$ -enamino ketones, which with NaOEt in DMF rearranged to imidazole derivs. E.g., I with (MeCO)<sub>2</sub>CH<sub>2</sub> gave II, which with NaOEt in DMF gave III. Condensation of I with PhCOCH<sub>2</sub>CO<sub>2</sub>Et gave IV and V. V was in solution equilibrium with its tautomer VI.

IT 55729-99-2P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 55729-99-2 CAPLUS

CN 1H-Imidazole-4-carboxylic acid, 2-(acetamino)-5-phenyl-, ethyl ester  
(9CI) (CA INDEX NAME)



ACCESSION NUMBER: 1962:46003 CAPLUS  
 DOCUMENT NUMBER: 56:46003  
 ORIGINAL REFERENCE NO.: 56:8702f-i,8703a-e  
 TITLE: 2-Phenylhydrazinoimidazoles and their benzidine-like rearrangement  
 AUTHOR(S): Pyl, Theodor; Lahmer, Helmut; Beyer, Hans  
 CORPORATE SOURCE: Univ. Greifswald, Germany  
 SOURCE: Chemische Berichte (1961), 94, 3217-23  
 CODEN: CHBEAM; ISSN: 0009-2940  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Unavailable  
 OTHER SOURCE(S): CASREACT 56:46003

AB PhNHC(:NH)NH<sub>2</sub> (I) reacts with BzCH<sub>2</sub>Br (II) and its aryl analogs to yield the corresponding 2-phenylhydrazinoimidazoles (III) which undergo with concentrated HCl a benzidine-like rearrangement. The structure was proved by the rearrangement of 2-phenylhydrazino-4(5)-phenylimidazole (IV) to 2-amino-4-phenyl-5-(p-aminophenyl)imidazole (V) and subsequent deamination to the known 2-amino-4,5-diphenylimidazole (VI). The lack of reducing properties in the III indicates the presence of the tautomeric 2-imidazolone phenylhydrazone form. I.HCl (3.73 g.) in 25 cc. MeOH treated with cooling with 0.46 g. Na in 20 cc. MeOH, filtered, and treated with 2 g. II in Me<sub>2</sub>CO gave 1.5 g. IV, needles, m. 225-6° (decomposition) (BuOH), turned yellow to pink in air; IV.HCl, rodlets, m. 201° (decomposition) (BuOH). IV refluxed 1 hr. with excess Ac<sub>2</sub>O in C<sub>5</sub>H<sub>5</sub>N gave the di-Ac derivative (VII) of IV, leaflets, m. 232° (decomposition) (1:1 BuOH-EtOH); di-Bz derivative, yellowish powder, decomposing above 230° with darkening. I.HCl (3.73 g.) and 2.78 g. p-BrC<sub>6</sub>H<sub>4</sub>COCH<sub>2</sub>Br gave 1.5 g. 4(5)-p-BrC<sub>6</sub>H<sub>4</sub> analog (VIII) of IV, needles, m. 227° (decomposition) (BuOH); VIII.HCl, rodlets, m. 215° (decomposition); di-Ac derivative of VIII, yellowish microcryst. powder, m. 155-6° (aqueous EtOH). I.HCl (3.73 g.) with 1.86 g. p-MeC<sub>6</sub>H<sub>4</sub>COCH<sub>2</sub>Cl gave 1.5 g. 4(5)-p-MeC<sub>6</sub>H<sub>4</sub> analog (IX) of IV, needles, m. 223-4°, (BuOH); IX.HCl, rodlets, m. 198° (decomposition); di-Ac derivative of IX, rodlets, m. 272-3° (aqueous EtOH). I.HCl (3.73 g.) with 2.3 g. p-MeOC<sub>6</sub>H<sub>4</sub>COCH<sub>2</sub>Br yielded 1.6 g. 4(5)-p-MeOC<sub>6</sub>H<sub>4</sub> analog of IV, needles, m. 215-16° (decomposition); IV.HCl, rodlets, m. 213-14° (decomposition) (BuOH); di-Ac derivative, yellowish crystal powder, m. 172-3°. IV (0.5 g.) in 3 cc. o-HOC<sub>6</sub>H<sub>4</sub>CHO refluxed briefly, cooled, diluted with 2 vols. EtOH, and filtered gave nearly 100% 4-phenyl-5-salicylidene-2-imidazolone phenylhydrazone (X), yellow needles, m. 230° (decomposition) (EtOH). Similarly were prepared the following 4-aryl analogs of X (aryl group and m.p. given): p-BrC<sub>6</sub>H<sub>4</sub> 213° (decomposition) (EtOH), p-MeC<sub>6</sub>H<sub>4</sub> 234° (decomposition) (EtOH); p-MeOC<sub>6</sub>H<sub>4</sub> 211° (decomposition) (EtOH); all yellow needles. VII (4 g.) and 40 cc. concentrated HCl refluxed 5 hrs., concentrated to beginning crystallization, cooled, and filtered gave 2 g. V.2HCl, needles, m. 310° (decomposition). IV (30 g.) and 250 cc. concentrated HCl refluxed, and the precipitate dissolved in a little H<sub>2</sub>O and repptd. with concentrated HCl gave 8 g. V.2HCl, needles, m. 310° (decomposition). V.2HCl in H<sub>2</sub>O treated with NH<sub>4</sub>OH gave V, yellowish rodlets, m. 265° (decomposition). V and excess Ac<sub>2</sub>O refluxed 1 hr. gave the di-Ac derivative, needles, m. 261° (EtOH). VIII (25 g.) in 250 cc. concentrated HCl refluxed 5 hrs., cooled, decanted from some resin, kept some time, filtered, and concentrated, and the precipitate dissolved in a little cold H<sub>2</sub>O and repptd. with concentrated HCl gave 3 g. 4-(p-BrC<sub>6</sub>H<sub>4</sub>) analog (X.2HCl) of V.2HCl, needles, m. 220° (decomposition). X.2HCl in H<sub>2</sub>O treated with dilute NH<sub>4</sub>OH gave X, powder, decomposing above 310° (aqueous EtOH). IX (26 g.) yielded similarly 8 g. 4-(p-MeC<sub>6</sub>H<sub>4</sub>) analog of

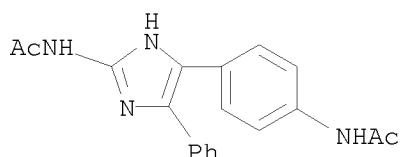
V. 2HCl, needles, m. 305°; free base, colorless prisms, decompose 303°; di-Ac derivative, yellowish crystal powder, m. 296° (EtOH). V (2 g.) in 5 cc. concentrated HCl and 50 cc. H2O treated at 0° with 0.6 g. NaNO2 in 5 cc. H2O and added to 1 g. 2-C10H7OH in 100 cc. 20% aqueous NaOH, and the violet flocculent precipitate washed with H2O, dissolved in 100 cc. hot EtOH, filtered, and diluted with H2O and a few drops HCl gave 0.8 g. 5-[p-(2-C10H7N:N)C6H4] analog of V, brown-violet powder, decomposing at higher temperature without melting, red-violet in organic solvents.

Diazotized V added to aqueous H3PO2, and the crystalline precipitate crystallized from dilute HCl, dissolved in MeOH, treated with dilute aqueous NaOH, and diluted with H2O yielded VI, prisms, m. 243° (decomposition).

IT 98783-56-3P, Acetanilide, 4'-[2-acetamido-5(or 4)-phenylimidazol-4-(or 5)-yl]- 99080-81-6P, Acetanilide, 4'-[2-acetamido-5(or 4)-p-tolylimidazol-4-(or 5)-yl]-  
 RL: PREP (Preparation)  
 (preparation of)

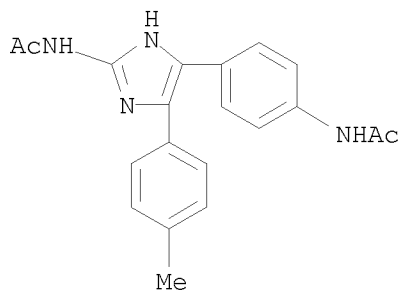
RN 98783-56-3 CAPLUS

CN Acetanilide, 4'-[2-acetamido-5(or 4)-phenylimidazol-4(or 5)-yl]- (7CI)  
 (CA INDEX NAME)



RN 99080-81-6 CAPLUS

CN Acetanilide, 4'-[2-acetamido-5(or 4)-p-tolylimidazol-4(or 5)-yl]- (7CI)  
 (CA INDEX NAME)



L15 ANSWER 24 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1919:6989 CAPLUS

DOCUMENT NUMBER: 13:6989

ORIGINAL REFERENCE NO.: 13:1301f-i,1302a-i,1303a-i,1304a-b

TITLE: Nitro-, arylazo-, and aminoglyoxalines

AUTHOR(S): Fargher, Robert George; Pyman, Frank Lee

CORPORATE SOURCE: Welcome Chem. Res. Lab., London

SOURCE: Journal of the Chemical Society, Transactions ( 1919), 115, 217-60  
 CODEN: JCHTA3; ISSN: 0368-1645

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB cf. C. A. 10, 1631. All m. ps. are corr. The object of this investigation was to prepare purine derivs. by building up a pyrimidine ring upon a glyoxaline nucleus, a method complementary to the usual one. It was proposed to prepare 4-aminoglyoxaline-5-carboxylic acid,  $\text{CH:N.C(NH}_2\text{):C(CO}_2\text{H).NH}$ , condense it with  $\text{HCNO}$  and obtain xanthine. The synthesis was not accomplished because of inability to obtain the starting material. I. The preparation of glyoxalines and their carboxylic acids: Glyoxaline-4,5-dicarboxylic acid (a), prepared in 60% yield by mixing cold aqueous solns. of nitrotartaric acid and  $\text{CH}_2\text{O}$ , m.  $288^\circ$  (decomposition). Mono-sodium salt, forms feathery needles containing 1  $\text{H}_2\text{O}$ . Glyoxaline (b) is prepared by distilling (a) in small quantities at a time; picrate, yellow needles containing 1  $\text{H}_2\text{O}$ , m.  $212^\circ$ ; hydrogen tartrate, anhydrous prisms, m.  $202^\circ$ ; hydrogen oxalate, anhydrous prismatic needles, m.  $232^\circ$ . On heating (a) to above  $180^\circ$  with  $\text{H}_2\text{O}$  or  $\text{HCl}$  the main product is (b) with a little glyoxaline-4-carboxylic acid. When (a) is heated to  $180\text{--}200^\circ$  with concentrated  $\text{NH}_4\text{OH}$  the main product is (b). On boiling (a) with  $\text{PhNH}_2$  the main product is glyoxaline-4-carboxanilide, anhydrous needles, m.  $227\text{--}8^\circ$ , hydrolyzed by 10%  $\text{HCl}$  at  $130^\circ$ , producing glyoxaline-4-carboxylic acid. 2-Methylglyoxaline-4,5-dicarboxylic acid (c) is prepared from  $\text{AcH}$  and nitrotartaric acid in 67% yield. On boiling (c) with  $\text{PhNH}_2$  there is obtained 11 g. 2-methyl-glyoxaline-4-carboxanilide (d), m.  $208^\circ$ , and 3.8 g. 2-methylglyoxaline; picrate, anhydrous needles from  $\text{H}_2\text{O}$ , m.  $213^\circ$ ; hydrogen oxalate, rhombic prisms from  $\text{H}_2\text{O}$  containing 2  $\text{H}_2\text{O}$ ; after drying at  $100^\circ$  it m.  $160^\circ$ . Hydrolysis of (d) gives 2-methylglyoxaline-4-carboxylic acid as a monohydrate, prismatic needles, m.  $262^\circ$  (decomposition); nitrate, rhombic prisms from  $\text{H}_2\text{O}$ , m.  $190^\circ$ ; picrate, minute cubes containing  $2\text{H}_2\text{O}$ , m.  $200^\circ$ . 2-Ethylglyoxaline-4,5-dicarboxylic acid, prepared from  $\text{EtCHO}$  and nitrotartaric acid in 64% yield, m.  $259^\circ$  (decomposition). 2-Phenylglyoxaline-4,5-dicarboxylic acid, from  $\text{BzH}$  and nitrotartaric acid in 48% yield, m.  $271^\circ$  (decomposition). When distilled in small quantities it gives an 80% yield of 2-phenylglyoxaline, needles from  $\text{H}_2\text{O}$ , m.  $148\text{--}9^\circ$ ; nitrate, leaflets from alc. containing 0.75  $\text{H}_2\text{O}$ , m. (dry)  $135^\circ$ ; hydrogen oxalate, needles, m.  $219^\circ$  (decomposition); picrate, fine needles, m.  $238^\circ$ . Upon mixing 8.6 g.  $\text{Ac}_2$  in 50 cc.  $\text{H}_2\text{O}$ , 50 cc. of 40% aqueous  $\text{CH}_2\text{O}$ , and 80 cc. concentrated  $\text{NH}_4\text{OH}$  at  $0^\circ$  there is obtained after standing in a cool place overnight, evaporating to a small bulk, saturating with  $\text{K}_2\text{CO}_3$ , extracting with  $\text{Et}_2\text{O}$ , and evaporating the extract, 5.9 g. of an oil which is boiled with dilute  $\text{HCl}$  to destroy  $\text{C}_6\text{H}_{12}\text{N}_4$  and separated by fractionating the picrates from  $\text{H}_2\text{O}$  into 5.7 g. 4,5-dimethylglyoxaline picrate (e), and 3.5 g. 2,4,5-trimethylglyoxaline picrate, m.  $163^\circ$ . 4,5-Dimethylglyoxaline hydrochloride forms rhombic prisms from  $\text{H}_2\text{O}$ , m.  $305^\circ$  (decomposition). (e) is also prepared from  $\text{MeCOC(:NOH)Me}$  (9 g.) by reducing with  $\text{SnCl}_2$  at  $15^\circ$  and evaporating the final liquor under reduced pressure; the resulting 10 g.  $\text{MeCOCH(NH}_2\text{)Me}$  heated on the  $\text{H}_2\text{O}$  bath 4 hrs. with 10 g.  $\text{KCNS}$  and 40 cc.  $\text{H}_2\text{O}$  gives 5.2 g. 2-thiol-4,5-dimethylglyoxaline and the latter gives an 85% yield of (e) when oxidized with the calculated quantity of  $\text{FeCl}_3$ . II. Nitroglyoxalines: 4-Nitroglyoxaline (f) is obtained in 63% yield when 8 g. of (b) in 16 cc. cold  $\text{HNO}_3$  (1.4), is cautiously treated with 16 cc.  $\text{H}_2\text{SO}_4$ , and after the vigorous reaction is over boiled 2 hrs. and poured into ice- $\text{H}_2\text{O}$ . 4-Nitro-2-methylglyoxaline, (g), prepared similarly, anhydrous needles from  $\text{H}_2\text{O}$ , sinter  $251^\circ$ , m.  $254^\circ$ . On nitrating 4-methylglyoxaline by the method of Windaus (C. A. 3, 1268) the main product is 4-methylglyoxaline nitrate instead of 5-nitro-4-methylglyoxaline (h) as stated by him. (h), obtained in 90% yield by the method described for preparing (g), m.  $248^\circ$ . On attempting to nitrate 4,5-dimethylglyoxaline (5 g.) with  $\text{HNO}_3$  and  $\text{H}_2\text{SO}_4$  1.7 g. was recovered

unchanged and the only product was 0.3 g. of the nitrate of 4-methylglyoxaline-5-carboxylic acid. When (f), (g), or (h) are reduced with Sn and HCl two of the three atoms of N present are eliminated as NH<sub>3</sub>. Three mols. (f) on reduction with alkaline Na<sub>2</sub>S<sub>2</sub>O<sub>4</sub> loses 2 atoms N as NH<sub>3</sub>. The remaining liquor gradually acquired a blue color as noted by Behrend and Schmitz (Ann. 277, 338) and on acidification precipitated less than 0.1 g.

of

a blue compound m. above 300°. (h) on reduction behaved analogously but gave a rose color and no precipitate (g) gave 1 mol. of NH<sub>3</sub> from 3 mols. of the nitro-compound III. Arylazoglyoxalines: In the opinion of the authors it appears that glyoxalines, in order to be capable of coupling, must contain a free « NH group and also a H atom or some other displaceable group, such as CO<sub>2</sub>H, in one of the 2-, 4-, or 5-positions. All previously prepared arylazoglyoxalines are C-azo compds. In general, the monoarylazoglyoxalines are soluble in alc., EtOAc and Me<sub>2</sub>CO, sparingly soluble in Et<sub>2</sub>O, CHCl<sub>3</sub> and C<sub>6</sub>H<sub>6</sub>, insol. in cold H<sub>2</sub>O and dilute alkali, form soluble salts with dilute HCl; are decomposed by boiling 1 hr. with 10% HCl, give bright colors with concentrated H<sub>2</sub>SO<sub>4</sub>. 17 g. (b) and 40 g. Na<sub>2</sub>CO<sub>3</sub> in 125 cc. H<sub>2</sub>O treated at 5° with a diazotized solution of 23.25 g. PhNH<sub>2</sub> give an orange powder which, on extracting with cold 2.5% HCl, left 4.4 g. residue of 2,4,5-trisbenzeneazoglyoxaline, decomp. about 200°, effervesces 208°. The HCl extract made alkaline gave 34 g. 2-benzeneazoglyoxaline (i), m. 190°. 20 g. of (i) reduced with SnCl<sub>2</sub> gives 3.2 g. 2-aminoglyoxaline, chlorostannate, a trace of NH<sub>2</sub>C(:NH)NH<sub>2</sub>, and 18.55 g. 2-amino-4-p-aminophenylglyoxaline dihydrochloride (j), formed by rearrangement of the benzidine type, m. above 300°; free base, formed by boiling with Na<sub>2</sub>CO<sub>3</sub>, glistening leaflets containing 1 H<sub>2</sub>O, m. 148°; dipicrate, yellow needles, darken 245°, M. 250° (decomposition). 2-Acetylaminoglyoxaline, by boiling the base with Ac<sub>2</sub>O 1 hr., crystalline powder, m. above 300°. 10 g. in dilute H<sub>2</sub>SO<sub>4</sub> with 4% KMnO<sub>4</sub> gave 1 g. p-AcNHC<sub>6</sub>H<sub>4</sub>CO<sub>2</sub>H, m. 260°. Reduction of 17.2 g. (i) with Zn dust and AcOH gives a small amount of (j), 7 g. PhNH<sub>2</sub>, and 5.9 g. of pure glycoylamidine hydrochloride (k), sintered 205°, m. 211-3°; free base, prismatic needles. begins darkening 220° and does not m. 300°; chloroplatinate, C<sub>3</sub>H<sub>5</sub>ON<sub>3</sub>.H<sub>2</sub>PtCl<sub>6</sub>.2H<sub>2</sub>O, darkens 220°, entirely black at 260°, does not m. 300°; chloraurate, C<sub>3</sub>H<sub>5</sub>ON<sub>3</sub>.AuCl<sub>3</sub>, m. 157-8°; picrate, yellow leaflets, m. 215-16°. By treating 13.6 g. (b) in Na<sub>2</sub>CO<sub>3</sub> at 5° with a diazotized solution of 34.4 g. p-BrC<sub>6</sub>H<sub>4</sub>NH<sub>2</sub> there resulted 48.7 g. crude 2-p-bromobenzeneazoglyoxaline (l); crystallization from alc. gave 42.6 g. of the pure compound m. 253° (decomposition) and a small amount of 4-p-bromobenzeneazoglyoxaline, m. 191° (decomposition). (l) (78 g.) on reduction with SnCl<sub>2</sub> gave 40.7 g. p-BrC<sub>6</sub>H<sub>4</sub>NH<sub>2</sub>, 2.7 g. of 2-amino-4-p-aminophenylglyoxaline, isolated as the picrate, 1.6 g. NH<sub>2</sub>C(:NH)NH<sub>2</sub>.(CO<sub>2</sub>H)<sub>2</sub>, m. 173-4°, 0.9 g. of a base forming needles, m. 178°, probably having the structure 5,2-Br(H<sub>2</sub>N)C<sub>6</sub>H<sub>3</sub>NHC:N.CH:CH.NH, and 20.7 g. 2-aminoglyoxaline hydrochloride (m), plates from alc., m. 152°; free base, obtained as a colorless sirup by adding 1 equivalent of Na<sub>2</sub>CO<sub>3</sub>, evaporating to dryness, extracting with alc., and evaporating the alc.; chlorostannate, prismatic needles, m. 286°; nitrate, transparent tablets, sinter 125°, m. 135-6°; hydrogen oxalate, tablets, m. 211°; picrate, silky needles, m. 236°. 2-Acetylaminoglyoxaline, prepared by boiling (m) with Ac<sub>2</sub>O and AcONa, prisms, sinter 270°, m. 287°. 2-Benzoylaminoglyoxaline, prepared by Schotten-Baumann reaction, leaflets, m. 227°. 4-Methylglyoxaline (32.8 g.) in NaHCO<sub>3</sub> treated with PhN:NC<sub>1</sub> gave 17.3 g. 2,5-bisbenzeneazo-4-methylglyoxaline, garnet-red needles from alc., m. 206° (decomposition); 17 g. of 5-benzeneazo-4-methylglyoxaline (n), copper-colored needles, m.

240° (decomposition); 7.4 g. of 2-benzeneazo-4-methylglyoxaline (o), orange prisms, m. 185°. Reduced with SnCl<sub>2</sub> (o) gives 2-amino-5-p-amixophenyl-4-methylglyoxaline dihydrochloride (p), diamond-shaped plates, m. above 300°. (p) boiled with Na<sub>2</sub>CO<sub>3</sub> gives the monohydrochloride, flat needles, sinter 80°, m. 260°; dipicrate, yellow needles, m. 255°.

2-Acetylamino-5-p-acetylaminophenyl-4-methylglyoxaline hydrochloride, prepared by the action of Ac<sub>2</sub>O and AcONa on (p), needles containing 4 H<sub>2</sub>O, after drying at 100° m. 303° (decomposition). On adding NH<sub>4</sub>OH to the solution of the hydrochloride the free base is precipitated, needles, m. 280°. 2-Amino-5-p-benzylideneaminophenyl-4-methylglyoxali neacetate, prepared by adding BzH to (p) in AcONa solution, m. 208°. (o) on reduction with Zn and AcOH gave 1.4 g. brown sirup from which was separated a small quantity of the dipicrate of (p) and about 0.7 g. alacreatinine hydrochloride, prisms, m. 202-3°; free base, m. 222-3°; picrale, yellow needles, sinter 200°, m. 212°. On reduction of 14 g. of (n) with SnCl<sub>2</sub> there is obtained besides PhNH<sub>2</sub> and a brown gum, 2.2 g. of the hydrochloride, C<sub>9</sub>H<sub>10</sub>N<sub>2</sub>.HCl, rectangular tablets, m. 308°, from which a base, C<sub>3</sub>H<sub>10</sub>N<sub>2</sub>, is obtained by adding NH<sub>4</sub>OH and crystallizing from H<sub>2</sub>O, prisms, m. 185°. Reduction of 10. g. (n) with Zn and AcOH produced 5.5 g. of a varnish-like substance and 1.6 g. of the base C<sub>10</sub>HON<sub>3</sub>, small, rhomboidal plates, m. 265°; hydrochloride, oblong plates, m. 206-8°, decomposed by heating 2.5 hrs. at 170° into NH<sub>4</sub>Cl and a hydrochloride, m. about 280°.

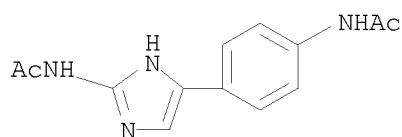
2-Methylglyoxaline in Na<sub>2</sub>CO<sub>3</sub> treated with PhN:NCl gives a product which easily resinifies and from which a small amount of 4-benzeneazo-2-methylglyoxaline was obtained pure, m. 158°.

4-p-Bromobenzeneazo-2-methylglyoxaline, prepared in good yield from 2-methylglyoxaline in Na<sub>2</sub>CO<sub>3</sub> and p-BrC<sub>6</sub>H<sub>4</sub>N:NCl, red prism sfrom absolute alc., m. 200° (decomposition); reduction with either SnCl<sub>2</sub> or Zn and AcOH give no definite products. 2-Phenylglyoxaline (7.2 g.) heated with p-BrC<sub>6</sub>H<sub>4</sub>N:NCl gives 13 g. 2-phenyl-4-p-bromobenzeneazoglyoxaline (q), orange needles, m. 201°. Reduction of (g) with SnCl<sub>2</sub> gives a crystalline hydrochloride, C<sub>15</sub>H<sub>13</sub>N<sub>4</sub>Br.2HCl, m. 255°; triacetyl derivative, formed by heating with Ac<sub>2</sub>O and AcONa, m. above 300°. This base is probably the result of a change of the semidine or benzidine type. 2-p-Sulfobenzeneazoglyoxaline-4,5-dicarboxylic acid, prepared by treating glyoxaline-4,5-dicarboxylic acid with SO<sub>3</sub>HC<sub>6</sub>H<sub>4</sub>N:NCl, red prisms containing 2 H<sub>2</sub>O which are lost at 130° in vacuo; disodium salt (r), yellow, silky needles containing 3 H<sub>2</sub>O. Reduction of 6.2 g. (r) with Na<sub>2</sub>S<sub>2</sub>O<sub>4</sub> gives 1.6 g. of 2-aminoglyoxaline-4,5-dicarboxylic acid, pale buff needles, effervesce 245° and then melt. On boiling 6 hrs. with PhNH<sub>2</sub> the product was identified as (m).

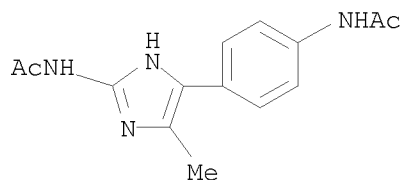
IT 861294-61-3P, Imidazole, 2-acetamido-4-(p-acetamidophenyl)-  
861325-21-5P, Imidazole, 2-acetamido-5-(p-acetamidophenyl)-4-  
methyl-, hydrochloride 861325-23-7P, Acetanilide,  
p-(2-acetamido-4-methyl-5-imidazolyl)-  
RL: PREP (Preparation)  
(preparation of)

RN 861294-61-3 CAPLUS

CN Acetamide, N-[4-[2-(acetylamino)-1H-imidazol-5-yl]phenyl]- (CA INDEX NAME)

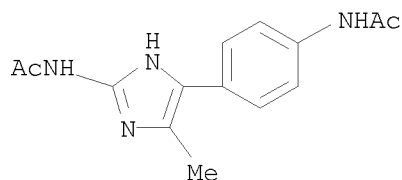


RN 861325-21-5 CAPLUS  
CN Acetamide, N-[4-[2-(acetylamino)-4-methyl-1H-imidazol-5-yl]phenyl]-,  
hydrochloride (1:1) (CA INDEX NAME)



● HCl

RN 861325-23-7 CAPLUS  
CN Acetamide, N-[4-[2-(acetylamino)-4-methyl-1H-imidazol-5-yl]phenyl]- (CA  
INDEX NAME)



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Uploading C:\Program Files\STNEXP\Queries\10564010 str 5.str

L18 STRUCTURE UPLOADED

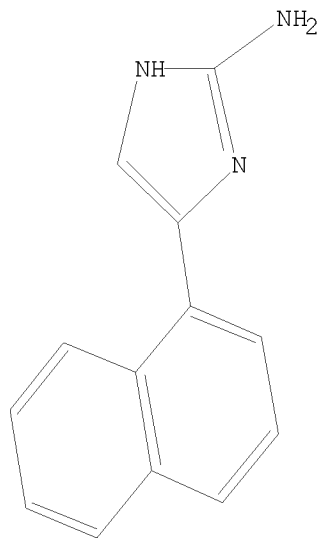
=> que L18

L19 QUE L18

=> d 119

L19 HAS NO ANSWERS

L18 STR



Structure attributes must be viewed using STN Express query preparation.

L19 QUE ABB=ON PLU=ON L18

=> s 119 sss full

FULL SEARCH INITIATED 11:55:21 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 599 TO ITERATE

100.0% PROCESSED 599 ITERATIONS 14 ANSWERS  
SEARCH TIME: 00.00.01

L20 14 SEA SSS FUL L18

=> file caplus

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FILE COVERS 1907 - 27 Oct 2008 VOL 149 ISS 18  
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SQN - Protein sequence name information, includes RN

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SQIDE - IDE, plus sequence data  
SQIDE3 - Same as SQIDE, but 3-letter amino acid codes are used  
SQD - Protein sequence data, includes RN

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PPROP - Table of predicted properties  
PROP - EPROP, ETAG, PPROP and SPEC

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FILE 'REGISTRY' ENTERED AT 11:30:38 ON 27 OCT 2008

L1 STRUCTURE UPLOADED  
L2 QUE L1  
L3 22 S L2 SSS FULL

FILE 'CAPLUS' ENTERED AT 11:31:05 ON 27 OCT 2008

L4 22 S L3  
L5 16 S L4 AND PY<=2004

FILE 'REGISTRY' ENTERED AT 11:40:27 ON 27 OCT 2008

L6 STRUCTURE UPLOADED  
L7 QUE L6  
L8 1 S L7 SSS FULL

FILE 'CAPLUS' ENTERED AT 11:40:57 ON 27 OCT 2008  
L9 0 S L8  
L10 0 S L8

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L11 STRUCTURE UPLOADED  
L12 QUE L11  
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L14 44 S L13  
L15 24 S L14 AND PY<=2004  
L16 0 S L15 AND 5-HYDROXYTRYPTAMINE  
L17 0 S L15 AND 5HT

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FILE 'REGISTRY' ENTERED AT 11:54:29 ON 27 OCT 2008  
L18 STRUCTURE UPLOADED  
L19 QUE L18  
L20 14 S L19 SSS FULL

FILE 'CAPLUS' ENTERED AT 11:55:38 ON 27 OCT 2008

FILE 'REGISTRY' ENTERED AT 11:55:51 ON 27 OCT 2008

FILE 'CAPLUS' ENTERED AT 11:55:58 ON 27 OCT 2008

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=> s 120

L21 12 L20

=> s 121 and py<=2004

25113423 PY<=2004

L22 3 L21 AND PY<=2004

=> d 122 1-3 ibib ab

L22 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:80450 CAPLUS

DOCUMENT NUMBER: 140:145835

TITLE: Preparation of dibenzofused  
bicyclo[2.2.2]octane-derived amides as modulators of  
the glucocorticoid receptor

INVENTOR(S): Vaccaro, Wayne; Yang, Bingwei Vera; Kim, Soong-hoon;  
Huynh, Tram; Tortolani, David R.; Leavitt, Kenneth J.;  
Li, Wenying; Doweiko, Arthur M.; Chen, Xiao-tao;  
Doweiko, Lidia

PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA; et al.

SOURCE: PCT Int. Appl., 265 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004009017	A2	20040129	WO 2003-US22300	20030717 <--
WO 2004009017	A3	20040708		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
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AU 2003251970	A1	20040209	AU 2003-251970	20030717 <--
US 20040132758	A1	20040708	US 2003-621909	20030717 <--
US 6995181	B2	20060207		
EP 1534273	A2	20050601	EP 2003-765638	20030717
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK			
JP 2006508042	T	20060309	JP 2004-523482	20030717
NO 2005000074	A	20050309	NO 2005-74	20050106
US 20050171136	A1	20050804	US 2005-85347	20050321
PRIORITY APPLN. INFO.:			US 2002-396877P	P 20020718
			US 2003-621909	A1 20030717
			WO 2003-US22300	W 20030717

OTHER SOURCE(S): MARPAT 140:145835

AB Title compds. I [R-R4 = H, alk(en/yn)yl, alkoxy, aryl, etc.; Z = carboxamido, alkylamino, etc.] are prepared For instance, 2-amino-4,5-dimethylthiazole is coupled to the acid derived from the

cycloaddn. of methacrylic acid and anthracene (CH<sub>3</sub>CN, EDCI, Et<sub>3</sub>N, HOAt, 18 h) to give II. I are glucocorticoid receptor modulators which are useful in treating diseases requiring glucocorticoid receptor agonist or antagonist therapy such as obesity, diabetes, inflammatory and immune disorders.

L22 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:80449 CAPLUS  
 DOCUMENT NUMBER: 140:157927  
 TITLE: Homology modeling of nuclear hormone receptor Site II and design of Site II ligands  
 INVENTOR(S): Doweiko, Arthur; Nadler, Steven G.  
 PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA  
 SOURCE: PCT Int. Appl., 276 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004009016	A2	20040129	WO 2003-US22299	20030717 <--
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
EP 1575502	A2	20050921	EP 2003-765637	20030717
EP 1575502	A3	20051123		
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK			
US 20060223110	A1	20061005	US 2003-621807	20030717
PRIORITY APPLN. INFO.:			US 2002-396907P	P 20020718
			WO 2003-US22299	W 20030717

AB A binding site in nuclear hormone receptors is described and its structural coordinates are provided. The invention provides machine-readable data storage media comprising structure coordinates of Site II and computer systems comprising the machine-readable data storage media. The invention provides methods used in the design and identification of ligands of Site II and of modulators of nuclear hormone receptors. The invention provides ligands of Site II, modulators of NHRs, pharmaceutical compns. comprising modulators of NHRs, methods of modulating NHRs, and methods of treating diseases by administering modulators of an NHR. Also provided are methods of designing mutants, mutant NHRs, Site II binding assays, and models of Site II.

L22 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1981:84008 CAPLUS  
 DOCUMENT NUMBER: 94:84008  
 ORIGINAL REFERENCE NO.: 94:13701a,13704a  
 TITLE: Synthesis and halogenation of some new 2-amino-4-substituted imidazoles and their possible use as pesticides  
 AUTHOR(S): Nath, J. P.; Mahapatra, G. N.  
 CORPORATE SOURCE: Dep. Chem., Ravenshaw Coll., Cuttack, 753 003, India

SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1980), 19B(6), 526-8  
CODEN: IJSBDB; ISSN: 0376-4699

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 94:84008

AB Eleven imidazoles I (R = Ph, substituted Ph,  $\alpha$ -,  $\beta$ -naphthyl, 2-thienyl; R1 = H) were prepared by cyclizing RAC with guanidine using Br as condensing agent. Halogenating I (R1 = H) gave I (R1 = Br, Cl). Both halogenated and nonhalogenated imidazoles exhibit antifungal activity against *Piricularia oryzae* and antibacterial activity against the common pathogenic bacteria, *Staphylococcus aureus* and *Escherichia coli*. Structure-activity relationship was also discussed.

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L22 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:80450 CAPLUS

DOCUMENT NUMBER: 140:145835

TITLE: Preparation of dibenzofused bicyclo[2.2.2]octane-derived amides as modulators of the glucocorticoid receptor

INVENTOR(S): Vaccaro, Wayne; Yang, Bingwei Vera; Kim, Soong-hoon; Huynh, Tram; Tortolani, David R.; Leavitt, Kenneth J.; Li, Wenying; Doweyko, Arthur M.; Chen, Xiao-tao; Doweyko, Lidia

PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA; et al.

SOURCE: PCT Int. Appl., 265 pp.  
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004009017	A2	20040129	WO 2003-US22300	20030717 <--
WO 2004009017	A3	20040708		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
AU 2003251970	A1	20040209	AU 2003-251970	20030717 <--
US 20040132758	A1	20040708	US 2003-621909	20030717 <--
US 6995181	B2	20060207		
EP 1534273	A2	20050601	EP 2003-765638	20030717
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK			
JP 2006508042	T	20060309	JP 2004-523482	20030717
NO 2005000074	A	20050309	NO 2005-74	20050106
US 20050171136	A1	20050804	US 2005-85347	20050321
PRIORITY APPLN. INFO.:			US 2002-396877P	P 20020718
			US 2003-621909	A1 20030717

OTHER SOURCE(S): MARPAT 140:145835

AB Title compds. I [R-R4 = H, alk(en/yn)yl, alkoxy, aryl, etc.; Z = carboxamido, alkylamino, etc.] are prepared For instance, 2-amino-4,5-dimethylthiazole is coupled to the acid derived from the cycloaddn. of methacrylic acid and anthracene (CH3CN, EDCI, Et3N, HOAt, 18 h) to give II. I are glucocorticoid receptor modulators which are useful in treating diseases requiring glucocorticoid receptor agonist or antagonist therapy such as obesity, diabetes, inflammatory and immune disorders.

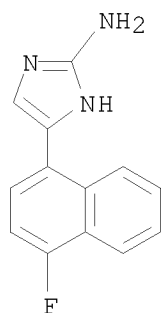
IT 650626-12-3 650626-16-7

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of dibenzofused bicyclo[2.2.2]octane-derived amides as modulators of glucocorticoid receptor)

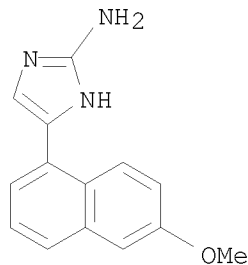
RN 650626-12-3 CAPLUS

CN 1H-Imidazol-2-amine, 5-(4-fluoro-1-naphthalenyl)- (CA INDEX NAME)



RN 650626-16-7 CAPLUS

CN 1H-Imidazol-2-amine, 5-(6-methoxy-1-naphthalenyl)- (CA INDEX NAME)



L22 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:80449 CAPLUS

DOCUMENT NUMBER: 140:157927

TITLE: Homology modeling of nuclear hormone receptor Site II and design of Site II ligands

INVENTOR(S): Doweyko, Arthur; Nadler, Steven G.

PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA

SOURCE: PCT Int. Appl., 276 pp.

CODEN: PIXXD2

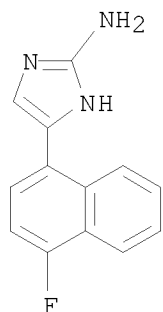
DOCUMENT TYPE: Patent

LANGUAGE: English

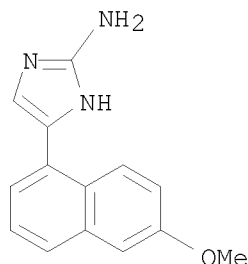
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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WO 2004009016	A2	20040129	WO 2003-US22299	20030717 <--
W:			AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW	
RW:			GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG	
EP 1575502	A2	20050921	EP 2003-765637	20030717
EP 1575502	A3	20051123		
R:			AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK	
US 20060223110	A1	20061005	US 2003-621807	20030717
PRIORITY APPLN. INFO.:			US 2002-396907P	P 20020718
			WO 2003-US22299	W 20030717
AB	A binding site in nuclear hormone receptors is described and its structural coordinates are provided. The invention provides machine-readable data storage media comprising structure coordinates of Site II and computer systems comprising the machine-readable data storage media. The invention provides methods used in the design and identification of ligands of Site II and of modulators of nuclear hormone receptors. The invention provides ligands of Site II, modulators of NHRs, pharmaceutical compns. comprising modulators of NHRs, methods of modulating NHRs, and methods of treating diseases by administering modulators of an NHR. Also provided are methods of designing mutants, mutant NHRs, Site II binding assays, and models of Site II.			
IT	650626-12-3P 650626-16-7P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (homol. modeling of nuclear hormone receptor Site II in ligand binding domain and design of Site II ligands)			
RN	650626-12-3 CAPLUS			
CN	1H-Imidazol-2-amine, 5-(4-fluoro-1-naphthalenyl)- (CA INDEX NAME)			



RN 650626-16-7 CAPLUS  
CN 1H-Imidazol-2-amine, 5-(6-methoxy-1-naphthalenyl)- (CA INDEX NAME)



L22 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1981:84008 CAPLUS

DOCUMENT NUMBER: 94:84008

ORIGINAL REFERENCE NO.: 94:13701a,13704a

TITLE: Synthesis and halogenation of some new  
2-amino-4-substituted imidazoles and their possible  
use as pesticides

AUTHOR(S): Nath, J. P.; Mahapatra, G. N.

CORPORATE SOURCE: Dep. Chem., Ravenshaw Coll., Cuttack, 753 003, India

SOURCE: Indian Journal of Chemistry, Section B: Organic  
Chemistry Including Medicinal Chemistry (1980  
, 19B(6), 526-8

CODEN: IJSBDB; ISSN: 0376-4699

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 94:84008

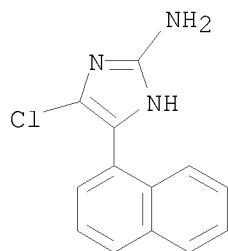
AB Eleven imidazoles I (R = Ph, substituted Ph,  $\alpha$ -,  $\beta$ -naphthyl,  
2-thienyl; R1 = H) were prepared by cyclizing RAc with guanidine using Br as  
condensing agent. Halogenating I (R1 = H) gave I (R1 = Br, Cl). Both  
halogenated and nonhalogenated imidazoles exhibit antifungal activity  
against *Piricularia oryzae* and antibacterial activity against the common  
pathogenic bacteria, *Staphylococcus aureus* and *Escherichia coli*.  
Structure-activity relationship was also discussed.

IT 76507-28-3P 76507-39-6P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation and pesticidal properties of)

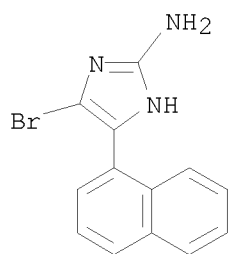
RN 76507-28-3 CAPLUS

CN 1H-Imidazol-2-amine, 5-chloro-4-(1-naphthalenyl)- (CA INDEX NAME)



RN 76507-39-6 CAPLUS

CN 1H-Imidazol-2-amine, 5-bromo-4-(1-naphthalenyl)- (CA INDEX NAME)



IT 76507-18-1P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation, halogenation and pesticidal properties of)

RN 76507-18-1 CAPLUS

CN 1H-Imidazol-2-amine, 5-(1-naphthalenyl)- (CA INDEX NAME)

